View metadata, citation and similar papers at core.ac.uk brought to you by CORE
provided by Publications Server of the Weierstrass Institute for Applied Analysis and Stochastics

SIAM J. MATH. ANAL.
Vol. 44, No. 6, pp. 3874–3900
© 2012 Society for Industrial and Applied Mathematics

# AN ELECTRONIC MODEL FOR SOLAR CELLS INCLUDING ACTIVE INTERFACES AND ENERGY RESOLVED DEFECT DENSITIES*

ANNEGRET GLITZKY†

**Abstract.** We introduce an electronic model for solar cells taking into account heterostructures with active interfaces and energy resolved volume and interface trap densities. The model consists of continuity equations for electrons and holes with thermionic emission transfer conditions at the interface and of ODEs for the trap densities with energy level and spatial position as parameters, where the right-hand sides contain generation-recombination as well as ionization reactions. This system is coupled with a Poisson equation for the electrostatic potential. We show the thermodynamic correctness of the model and prove a priori estimates for the solutions to the evolution system. Moreover, existence and uniqueness of weak solutions of the problem are proven. For this purpose we solve a regularized problem and verify bounds of the corresponding solution not depending on the regularization level.

**Key words.** reaction-diffusion systems, drift-diffusion processes, active interfaces, energy resolved defect densities, existence, uniqueness, a priori estimates

**AMS subject classifications.** 35K57, 35R05, 35B45, 78A35

**DOI.** 10.1137/110858847

**1. Introduction and notation.** This paper is devoted to the analysis of electronic models for solar cells including active interfaces, which take into account energy resolved defect (trap) densities. Different kinds of such traps occur in the bulk material and others live only at interfaces. These traps are assumed to be immobile, but during the time being they can change their charge states by reactions with bulk electrons and holes from both sides of the interface. Additionally thermionic emission effects for electrons and holes at the interface are taken into account.

Semiconductor models with varying in time densities of ionized impurities, where the impurities are associated to a fixed energy level have been investigated in [12]. Recently, in [9], we investigated a model with energy resolved defect densities in the bulk. But there no active interfaces (and no traps at interfaces) that were taken into account.

Our equations are based on models proposed by engineers working on solar cells (see, e.g., [20, sect. 4.2]). But, for an easier writing we consider the situation of only one kind of volume defect and one kind of interface defect. We demonstrate in this example how such defects can be analytically treated. Since there is only a very weak coupling of the effects of the different defects, our ideas can easily be generalized, to any finite number of kinds of defects in the bulk and at interfaces.

Moreover, we study here a special geometric situation of a heterostructure, which can be generalized to more complicated geometries. $\Omega \subset \mathbb{R}^2$ denotes the solar cell domain. The boundary $\partial\Omega$ of $\Omega$ splits into a part $\Gamma_D$, representing the contacts of the device and a part $\Gamma_N$, where the device is insulated. Let a hypersurface $\Gamma$ representing

*Received by the editors December 13, 2011; accepted for publication (in revised form) August 6, 2012; published electronically November 8, 2012. This work was partially supported by the DFG Research Center MATHEON "Mathematics for Key Technologies" under project D22.
http://www.siam.org/journals/sima/44-6/85884.html
†Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstrasse 39, D-10117 Berlin, Germany (glitzky@wias-berlin.de).



Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

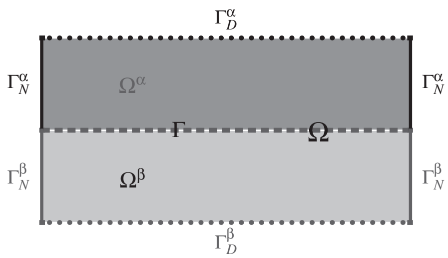


FIG. 1.1. *Heterostructure* $\Omega$ *with interface* $\Gamma$.

the active interface divide $\Omega$ into the two parts $\Omega^\alpha$ and $\Omega^\beta$ (see Figure 1.1). We assume that the active interface $\Gamma$ and the part of $\partial\Omega$, where Dirichlet conditions are prescribed, are strictly separated, that means $\inf_{x\in\Gamma_D,\, y\in\Gamma}|x-y| \geq \kappa_0 > 0$. We denote $\Gamma_D^\gamma = \Gamma_D \cap \bar{\Omega}^\gamma$, $\Gamma_N^\gamma = \partial\Omega^\gamma \setminus (\bar{\Gamma} \cup \bar{\Gamma}_D)$, $\gamma = \alpha, \beta$. Note that $\Gamma_D^\gamma$ is allowed to be empty for one $\gamma$.

For the analysis we rescale the quantities, such that energies are counted in units of $k_BT$, where $k_B$ is Boltzmann's constant and $T$ is the temperature. In this energy scale for $E \in E_G = [E_1, E_2]$ we take into account one kind of bulk (volume) defect with given defect distribution $N(x, E)$. To also include measure valued distributions of traps on the energy scale we use a finite nonnegative measure $\mu = N\mathrm{d}E$ on $G := \Omega \times E_G$ proposing Young measure type properties such that $\mu(x, \cdot)$ is a Radon measure on $E_G$ almost everywhere (a.e.) on $\Omega$ and $x \mapsto \int_{E_G} g(E)\mu(x, \mathrm{d}E)$ is measurable for all continuous functions $g : E_G \to \mathbb{R}$.

This setting allows for $\mu(x, \cdot) = \sum_{k=1}^K \theta_k(x)\delta_{E_k(x)}(\cdot)$ such that the case of point-like distributed traps at single energies $E_{trap} \in E_G$ as discussed in [12] result as special case of our investigations, too.

Additionally we consider one type of interface defects with distribution $N_\Gamma(x, E)$. Similarly we work with a finite nonnegative measure $\mu_\Gamma = N_\Gamma \mathrm{d}E$ on $G_\Gamma := \Gamma \times E_G$.

We use the abbreviations

$$\langle\langle g\rangle\rangle := \int_{E_G} g(E)\mu(x, \mathrm{d}E), \quad \langle\langle g\rangle\rangle_\Gamma := \int_{E_G} g(E)\mu_\Gamma(x, \mathrm{d}E).$$

Besides the densities of electrons $u_1$ and holes $u_2$ depending only on the spatial position $x$, we have to balance the following quantities: The probability that defect states with defect distribution $N(x, E)$ are occupied by an electron can be interpreted as the density of defects occupied by electrons on $G = \Omega \times E_G$ with respect to the measure $\mu$. We denote it by $u_3$, and $u_4 = 1 - u_3$ corresponds to the density of non-occupied defect states with respect to the measure $\mu$. Correspondingly we denote the density of interfacial defects occupied by electrons on $G_\Gamma = \Gamma \times E_G$ with respect to the measure $\mu_\Gamma$ by $u_{\Gamma 1}$, and $u_{\Gamma 2} = 1 - u_{\Gamma 1}$ corresponds to the density of nonoccupied defect states with respect to the measure $\mu_\Gamma$.

Moreover, we introduce the charge numbers of electrons, holes, volume, and interface traps,

$$\lambda_1 = -1, \quad \lambda_2 = 1, \quad \lambda_3 = \begin{cases} -1 & \text{for acceptor like traps,} \\ 0 & \text{for donator like traps,} \end{cases} \quad \lambda_4 = \lambda_3 + 1,$$

$$\lambda_{\Gamma 1} = \begin{cases} -1 & \text{for acceptor like traps,} \\ 0 & \text{for donator like traps,} \end{cases} \quad \lambda_{\Gamma 2} = \lambda_{\Gamma 1} + 1,$$

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

and use the vector $\lambda = (\lambda_1, \ldots, \lambda_4, \lambda_{\Gamma 1}, \lambda_{\Gamma 2}) \in \mathbb{R}^6$. In the bulk we consider capture/escape reactions of electrons from the conduction band by unoccupied traps and of holes from the valence band by occupied traps (see $R_1$, $R_2$ in (1.5)). Also the interface defects capture and escape charge carriers from $\Omega^\gamma$, see reaction rates $R_1^\Gamma$, $R_2^\Gamma$, $\gamma = \alpha, \beta$ in (1.5)).

The electronic model for solar cells with active interface proposed in [20] is a drift-diffusion model for the charge carriers coupled with ODEs for the defect occupation probabilities in the bulk $u_3(x,E)$, $u_4(x,E)$, $(x,E) \in G$ and with ODEs for the defect occupation probabilities at the interface $u_{\Gamma 1}(x,E)$, $u_{\Gamma 2}(x,E)$, $(x,E) \in G_\Gamma$. Additionally there occur transfer conditions at the interface including thermionic emission of electrons and holes. The incident light, generating pairs of electrons and holes, is treated as a given (time dependent) source term $G_{phot}$ in the continuity equations for electrons and holes. Let $z$ denote the scaled electrostatic potential and let $u_i = (u_i^\alpha, u_i^\beta)$ be the carrier densities with $u_i^\gamma$ being defined on $\overline{\Omega^\gamma}$, $\gamma = \alpha, \beta$, $i = 1, 2$. In our notation, the model proposed in [20, sect. 4.2] can be written as the drift-diffusion system

$$\begin{aligned}
&-\nabla \cdot (\varepsilon \nabla z) = f - u_1 + u_2 + \sum_{i=3}^{4} \lambda_i \langle\langle u_i \rangle\rangle + \delta_\Gamma \sum_{i=1}^{2} \lambda_{\Gamma i} \langle\langle u_{\Gamma i} \rangle\rangle_\Gamma \quad \text{in } \mathbb{R}_+ \times \Omega, \\
&\frac{\partial}{\partial t} u_i^\gamma + \nabla \cdot j_i^\gamma = G_{phot} - R - \langle\langle R_i \rangle\rangle \quad \text{in } \mathbb{R}_+ \times \Omega^\gamma, \quad \gamma = \alpha, \beta, \ i = 1, 2,
\end{aligned} \tag{1.1}$$

the ODEs

$$\frac{\partial}{\partial t} u_3 = R_1 - R_2, \quad \frac{\partial}{\partial t} u_4 = -\frac{\partial}{\partial t} u_3 \quad \text{on } \mathbb{R}_+ \times \operatorname{supp} \mu, \tag{1.2}$$

the ODEs at the interface

$$\frac{\partial}{\partial t} u_{\Gamma 1} = \sum_{\gamma = \alpha, \beta} \Big( R_{\Gamma 1}^\gamma - R_{\Gamma 2}^\gamma \Big), \quad \frac{\partial}{\partial t} u_{\Gamma 2} = -\frac{\partial}{\partial t} u_{\Gamma 1} \quad \text{on } \mathbb{R}_+ \times \operatorname{supp} \mu_\Gamma, \tag{1.3}$$

and the transfer conditions at the interface

$$\begin{aligned}
-j_i^\alpha \cdot \nu^\alpha &= \sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta + \langle\langle R_{\Gamma i}^\alpha(\cdot, u_i^\alpha, u_{\Gamma 1}, u_{\Gamma 2}) \rangle\rangle_\Gamma, \\
-j_i^\beta \cdot \nu^\beta &= \sigma_i^\beta u_i^\beta - \sigma_i^\alpha u_i^\alpha + \langle\langle R_{\Gamma i}^\beta(\cdot, u_i^\beta, u_{\Gamma 1}, u_{\Gamma 2}) \rangle\rangle_\Gamma \quad \text{on } \mathbb{R}_+ \times \Gamma, \quad i = 1, 2.
\end{aligned} \tag{1.4}$$

The flux terms and reaction rates in the continuity equations are given by

$$\begin{aligned}
j_i^\gamma &= -D_i(\nabla u_i^\gamma + \lambda_i u_i^\gamma \nabla z), \quad \gamma = \alpha, \beta, \ i = 1, 2, \\
R &= R(u_1, u_2) = r_0(u_1, u_2)[u_1 u_2 - k_0], \\
R_1 &= R_1(E, u_1, u_3, u_4) = r_1[u_1 u_4 - k_1 u_3], \\
R_2 &= R_2(E, u_2, u_3, u_4) = r_2[u_2 u_3 - k_2 u_4], \\
R_{\Gamma 1}^\gamma &= R_{\Gamma 1}^\gamma(E, u_1^\gamma, u_{\Gamma 1}, u_{\Gamma 2}) = r_{\Gamma 1}^\gamma[u_1^\gamma u_{\Gamma 2} - k_{\Gamma 1}^\gamma u_{\Gamma 1}], \\
R_{\Gamma 2}^\gamma &= R_{\Gamma 2}^\gamma(E, u_2^\gamma, u_{\Gamma 1}, u_{\Gamma 2}) = r_{\Gamma 2}^\gamma[u_2^\gamma u_{\Gamma 1} - k_{\Gamma 2}^\gamma u_{\Gamma 2}],
\end{aligned} \tag{1.5}$$

where the positive coefficients $r_0$, $k_0$ are allowed to depend in a nonsmooth way on the spatial position and the positive coefficients $r_i$, $k_i$, $r_{\Gamma i}^\gamma$, $k_{\Gamma i}^\gamma$, $\gamma = \alpha, \beta$, $i = 1, 2$, depend on $(x, E)$. In the Poisson equation, $f$ means a fixed doping profile and $\delta_\Gamma$ denotes the surface measure on $\Gamma$ such that, in the sense of distributions, $\int_\Omega w \delta_\Gamma v \, dx = \int_\Gamma w v \, da$ for all test functions $v$.

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

For the Poisson equation on $\partial\Omega$ we suppose

$$z = z^D \text{ on } \mathbb{R}_+ \times \Gamma_D, \quad \nu \cdot (\varepsilon \nabla z) = 0 \text{ on } \mathbb{R}_+ \times \Gamma_N. \tag{1.6}$$

For the continuity equations for $u_i^\gamma$ besides the transfer conditions (1.4) we assume that

$$u_i^\gamma = u_i^{\gamma D} \text{ on } \mathbb{R}_+ \times \Gamma_D^\gamma, \quad \nu \cdot j_i^\gamma = 0 \text{ on } \mathbb{R}_+ \times \Gamma_N^\gamma, \quad \gamma = \alpha, \beta,\ i = 1, 2. \tag{1.7}$$

We complete the model equations by initial conditions for the densities of all species

$$u_i(0) = U_i, \quad i = 1, \dots, 4, \quad u_{\Gamma i} = U_{\Gamma_i}, \quad i = 1, 2. \tag{1.8}$$

We introduce reference quantities $\widetilde{u}_3$, $\widetilde{u}_4$, $\widetilde{u}_{\Gamma 1}$, $\widetilde{u}_{\Gamma 2}$ fulfilling

$$u_1^D \widetilde{u}_4 = k_1 \widetilde{u}_3 \quad \mu\text{-a.e. in } G, \quad u_1^{\alpha D} \widetilde{u}_{\Gamma 2} = k_{\Gamma 1}^\alpha \widetilde{u}_{\Gamma 1} \quad \mu_\Gamma\text{-a.e. in } G_\Gamma.$$

*Remark.* Our model is an extensive generalization of the classical van Roosbroeck system [21] describing charge transport in semiconductor devices due to drift and diffusion within a self-consistent electrical field. First, mathematical analysis for this transient system was done in [18]; for more references, see [5]. Recently, [22] investigated existence and asymptotic behavior of solutions for the whole space situation. Global existence and uniqueness of weak solutions under physically realistic conditions in two space dimensions is achieved in [6]. In [14] the van Roosbroeck system is reformulated as an evolution equation for the potentials. In this setting a unique, local in time solution in Lebesgue spaces is available and leads to classical solutions to the drift-diffusion equations in the two-dimensional case. To handle the electronic model for solar cells including active interfaces, we profit from techniques approved for the van Roosbroeck system and combine them with new ideas.

The plan of this paper is the following: In section 2 we collect our general assumptions and give a weak formulation (P) of the electronic model for solar cells including active interfaces. Section 3 is devoted to a priori estimates for solutions to (P). In subsection 3.1 we start with energy estimates and establish $L^\infty$-estimates for solutions to (P) in subsection 3.2. Section 4 contains the existence and uniqueness proof for (P). In subsection 4.1 we introduce a regularized problem ($\mathrm{P}_M$) and prove its solvability in subsection 4.2. After deriving energy estimates (subsection 4.3) and $L^\infty$-estimates for solutions to ($\mathrm{P}_M$) (subsection 4.4) which are independent on the regularization level $M$, in subsection 4.5 the existence and uniqueness result for (P) is shown.

## 2. Assumptions and weak formulation.

**2.1. Assumptions. Some notation.** Let $\Omega \subset \mathbb{R}^2$ be a bounded Lipschitzian domain. The notation of function spaces in the present paper corresponds to that in [15]. To specify norms, we write $\|\cdot\|_{L^p}$ and $\|\cdot\|_{H^1}$ instead of $\|\cdot\|_{L^p(\Omega)}$ and $\|\cdot\|_{H^1(\Omega)}$. Moreover, let $\Gamma_N$, $\Gamma_D$ be disjoint open subsets of $\partial\Omega$ with $\partial\Omega = \overline{\Gamma_N} \cup \overline{\Gamma_D}$, where $\Gamma_0 := \overline{\Gamma_N} \cap \overline{\Gamma_D}$ consists of finitely many points. Let $\Omega \cup \Gamma_N$ be regular in the sense of Gröger [13]. For $1 \le p \le \infty$ we define $W_0^{1,p}(\Omega \cup \Gamma_N)$ as the closure of the set

$$\{w|_\Omega : w \in C^\infty(\mathbb{R}^2), (\Gamma_D \cup \Gamma_0) \cap \operatorname{supp}(w) = \emptyset\}$$

in $W^{1,p}(\Omega)$ equipped with the usual norm of the space $W^{1,p}(\Omega)$. Its dual is denoted by $W^{-1,p'}(\Omega \cup \Gamma_N)$, where $1/p + 1/p' = 1$; see [13]. Correspondingly, we use $H_0^1(\Omega \cup \Gamma_N)$.

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

For a Banach space $B$ we denote by $B_+$ the cone of nonnegative elements and by $B^*$ its dual space. We write $u^+$ ($u^-$) for the positive (negative) part of a function $u$. The abbreviation a.e. means $\mathcal{L}^d$-a.e., for the measures $\mu$ and $\mu_\Gamma$ we write $\mu$-a.e. and $\mu_\Gamma$-a.e. The scalar product in $\mathbb{R}^d$ is indicated by a centered dot. Positive constants which depend only on the data of our problem are denoted by $c$.

We collect the general assumptions our analytical investigations are based on.

(A1) $\Omega$, $\Omega^\alpha, \Omega^\beta \subset \mathbb{R}^2$ are bounded Lipschitzian domains, $\Gamma_D$, $\Gamma_N$ are disjoint open subsets of $\partial\Omega$, $\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_0$, and mes $\Gamma_D > 0$, and $\Gamma_0$ consists of finitely many points ($\Omega \cup \Gamma_N$ is regular in the sense of Gröger [13]). A part $\Gamma$ of a hypersurface devides $\Omega$ into Lipschitzian domains $\Omega^\alpha$ and $\Omega^\beta$, $\inf_{x\in\Gamma_D,\, y\in\Gamma} |x-y| \geq \kappa_0 > 0$, $\Gamma_D^\gamma = \Gamma_D \cap \bar{\Omega}^\gamma$, $\Gamma_N^\gamma = \partial\Omega^\gamma \setminus (\bar{\Gamma} \cup \bar{\Gamma}_D)$, $\gamma = \alpha, \beta$;

(A2) $N$ and $N_\Gamma$ generate finite nonnegative measures $\mu = N\mathrm{d}E$ on $G$ and $\mu_\Gamma = N_\Gamma \mathrm{d}E$ on $G_\Gamma$ such that $\mu(x,\cdot)$ and $\mu_\Gamma(x,\cdot)$ are Radon measures on $E_G$ a.e. on $\Omega$ and $\Gamma$, respectively. $x \mapsto \int_{E_G} g(E)\mu(x,\mathrm{d}E)$ and $x \mapsto \int_{E_G} g(E)\mu_\Gamma(x,\mathrm{d}E)$ are measurable for all continuous functions $g:\, E_G \to \mathbb{R}$, $\int_{E_G} \mu(x,\mathrm{d}E) \leq \hat{c}$ a.e. in $\Omega$, $\int_{E_G} \mu_\Gamma(x,\mathrm{d}E) \leq \hat{c}$ a.e. on $\Gamma$;

(A3) $G_{phot} \in L^\infty(\mathbb{R}_+, L_+^\infty(\Omega))$, $\|G_{phot}(t)\|_{L^\infty} \leq c$ for almost all (f.a.a.) $t \in \mathbb{R}_+$, $k_0 \in L_+^\infty(\Omega)$, $k_0 \geq c > 0$ a.e., $r_0 : \Omega \times \mathbb{R}_+^2 \to \mathbb{R}_+$, $r_0(x,\cdot)$ Lipschitzian, uniformly with respect to (w.r.t.) $x \in \Omega$, $r_0(\cdot,y)$ measurable for all $y \in \mathbb{R}_+^2$, $r_0(\cdot,0) \in L^\infty(\Omega)$, $r_i$, $k_i \in L_+^\infty(G;\mathrm{d}\mu)$, $k_i \geq c > 0$ $\mu$-a.e. on $G$, $r_{\Gamma i}^\gamma$, $k_{\Gamma i}^\gamma \in L_+^\infty(G_\Gamma;\mathrm{d}\mu_\Gamma)$, $k_{\Gamma i}^\gamma \geq c > 0$ $\mu_\Gamma$-a.e. on $G_\Gamma$, $\sigma_i^\gamma \in L_+^\infty(\Gamma)$, $\gamma = \alpha, \beta$, $i = 1, 2$;

(A4) $\varepsilon \in L^\infty(\Omega)$, $\varepsilon \geq c > 0$ a.e. on $\Omega$, $f \in L^2(\Omega)$, $z^D \in W^{1,\infty}(\Omega)$, $z^D|_{\Gamma_D} = z^D$ (cf. (1.6));

(A5) $D_i \in L^\infty(\Omega)$, $D_i \geq \epsilon > 0$ a.e. on $\Omega$, $i = 1, 2$, $u^D = ((u_1^{\alpha D}, u_1^{\beta D}), (u_2^{\alpha D}, u_2^{\beta D}), 0, 0, 0, 0)$, $\ln u_i^{\gamma D} \in W^{1,\infty}(\Omega^\gamma)$, with $u_i^{\gamma D}|_{\Gamma_D^\gamma} = u_i^{\gamma D}$ (cf. (1.7)), $u_i^{\gamma D}|_\Gamma = \frac{1}{\sigma_i^\gamma}$, $\gamma = \alpha, \beta$, $i = 1, 2$, $\widetilde{u}_i \in L^\infty(G, \mathrm{d}\mu)$, $\widetilde{u}_i \geq c > 0$, $i = 3, 4$, $u_1^D \widetilde{u}_4 = k_1 \widetilde{u}_3$ $\mu$-a.e. in $G$, $\widetilde{u}_{\Gamma i} \in L^\infty(G_\Gamma, \mathrm{d}\mu_\Gamma)$, $\widetilde{u}_{\Gamma i} \geq c > 0$, $i = 1, 2$, $u_1^{\alpha D} \widetilde{u}_{\Gamma 2} = k_{\Gamma 1}^\alpha \widetilde{u}_{\Gamma 1}$ $\mu_\Gamma$-a.e. in $G_\Gamma$;

(A6) $U_i \in L_+^\infty(\Omega)$, $i = 1, 2$, $U_3, U_4 \in L_+^\infty(G;\mathrm{d}\mu)$, $U_3, U_4 \leq 1$, $U_3 + U_4 = 1$ $\mu$-a.e. on $G$, $U_{\Gamma 1}$, $U_{\Gamma 2} \in L_+^\infty(G_\Gamma;\mathrm{d}\mu_\Gamma)$, $U_{\Gamma 1}$, $U_{\Gamma 2} \leq 1$, $U_{\Gamma 1} + U_{\Gamma 2} = 1$ $\mu_\Gamma$-a.e. on $G_\Gamma$.

*Remark* (physical relevance of our assumptions). Assumption (A1) describes a prototype situation of a heterostructure with an active interface in two dimensions (2D); for generalizations, see section 5. The Gröger regularity of $\Omega \cup \Gamma_N$ (whole domain) and the Lipschitz property for the subdomains $\Omega^\gamma$ are no real restrictions. The assumption (A2) allows us to consider traps with realistic physically motivated energy distributions. Particularly, the following situations are allowed: point like distributed at single energy, constantly distributed in a specific region of the band gap, and exponential decaying from the conduction/valence band into the band gap, and Gaussian distributed within the band gap. The assumption concerning $r_0$ are formulated in this weak form to include Shockley–Read–Hall as well as Auger generation/recombination processes. Moreover, we explicitely do not assume that for all considered processes

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

a detailed simultaneous equilibrium exists. This fits the physical relevant situation under consideration.

**2.2. Weak formulation.** We use the vector $U = (U_1, \dots, U_4, U_{\Gamma 1}, U_{\Gamma_2})$ and introduce the function spaces

$$\begin{aligned}
&Y := L^2(\Omega)^2 \times L^2(G; \mathrm{d}\mu)^2 \times L^2(G_\Gamma; \mathrm{d}\mu_\Gamma)^2, \qquad\qquad Z := H_0^1(\Omega \cup \Gamma_N),\\
&V := L^\infty(\Omega)^2 \times L^\infty(G; \mathrm{d}\mu)^2 \times L^\infty(G_\Gamma; \mathrm{d}\mu_\Gamma)^2,\\
&X := \big\{u = (u_1, \dots, u_4, u_{\Gamma 1}, u_{\Gamma 2}) \in Y\colon\\
&\qquad\qquad u_i = (u_i^\alpha, u_i^\beta),\ u_i^\gamma \in H^1(\Omega^\gamma), u_i^\gamma|_{\Gamma_D^\gamma} = 0,\ \gamma = \alpha, \beta,\ i = 1, 2\big\},
\end{aligned}$$

and define the operators $\mathcal{A}\colon [(X+u^D)\cap V_+]\times(Z+z^D)] \to X^*$, $\mathcal{R}\colon [X+u^D]\cap V_+ \to X^*$, and $\mathcal{P}\colon (Z + z^D) \times Y \to Z^*$ by

$$\begin{aligned}
\langle \mathcal{A}(u, z), \widehat{u}\rangle_X &:= \sum_{i=1}^2 \int_\Omega D_i(\nabla u_i + \lambda_i u_i \nabla z) \cdot \nabla \widehat{u}_i \,\mathrm{d}x, \quad \widehat{u} \in X,\\
\langle \mathcal{R}(u), \widehat{u}\rangle_X &:= \sum_{i=1}^2 \int_\Omega \big\{r_0(u_1u_2 - k_0) - G_{phot}\big\}\, \widehat{u}_i \,\mathrm{d}x\\
&\quad + \int_G \Big\{r_1(u_1u_4 - k_1u_3)(\widehat{u}_1{+}\widehat{u}_4{-}\widehat{u}_3)\\
&\quad + r_2(u_2u_3 - k_2u_4)(\widehat{u}_2{+}\widehat{u}_3{-}\widehat{u}_4)\Big\}\,\mathrm{d}\mu\\
&\quad + \sum_{\gamma=\alpha,\beta} \int_{G_\Gamma} \Big\{r^\gamma_{\Gamma 1}(u^\gamma_1 u_{\Gamma 2} - k^\gamma_{\Gamma 1} u_{\Gamma 1})(\widehat{u}^\gamma_1 + \widehat{u}_{\Gamma 2} - \widehat{u}_{\Gamma 1})\\
&\quad + r^\gamma_{\Gamma 2}(u^\gamma_2 u_{\Gamma 1} - k^\gamma_{\Gamma 2} u_{\Gamma 2})(\widehat{u}^\gamma_2 + \widehat{u}_{\Gamma 1} - \widehat{u}_{\Gamma 2})\Big\}\,\mathrm{d}\mu_\Gamma\\
&\quad + \sum_{i=1}^2 \int_\Gamma (\sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta)(\widehat{u}_i^\alpha - \widehat{u}_i^\beta)\,\mathrm{d}a, \quad \widehat{u} \in X,\\
\langle \mathcal{P}(z, u), \widehat{z}\rangle_Z &:= \int_\Omega \left\{\varepsilon \nabla z \cdot \nabla \widehat{z} - \left[f + \sum_{i=1}^2 \lambda_i u_i\right] \widehat{z}\right\} \mathrm{d}x - \sum_{i=3}^4 \int_G \lambda_i u_i \widehat{z}\,\mathrm{d}\mu\\
&\quad - \sum_{i=1}^2 \int_{G_\Gamma} \lambda_{\Gamma i} u_{\Gamma i} \widehat{z}\,\mathrm{d}\mu_\Gamma, \quad \widehat{z} \in Z.
\end{aligned}$$

Note that here integrals over $\Omega$ of expressions containing $u_1$, $u_2$ or $\nabla u_1$, $\nabla u_2$ take into account the values of $u_i^\gamma$ or $\nabla u_i^\gamma$ on $\Omega^\gamma$, $i = 1, 2$. Then the weak formulation of the electronic model for solar cells with active interfaces (1.1)–(1.8) reads as

$$\text{(P)} \qquad \left\{\begin{array}{c}
u'(t) + \mathcal{A}(u(t), z(t)) + \mathcal{R}(u(t)) = 0, \quad \mathcal{P}(z(t), u(t)){=}0, \quad \text{f.a.a. } t > 0,\\
u(0) = U, \quad u \in H^1_{\mathrm{loc}}(\mathbb{R}_+, X^*) \cap L^\infty_{\mathrm{loc}}(\mathbb{R}_+, V_+),\\
u - u^D \in L^2_{\mathrm{loc}}(\mathbb{R}_+, X), \quad z - z^D \in L^2_{\mathrm{loc}}(\mathbb{R}_+, Z) \cap L^\infty_{\mathrm{loc}}(\mathbb{R}_+, L^\infty(\Omega)).
\end{array}\right.$$

## 3. A priori estimates.

**3.1. Energy estimates.** To prove the thermodynamic correctness of the model we need three preparatory lemmas.

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Lemma 3.1. *We presume assumptions* (A1), (A2), (A4). *For any* $u \in Y$ *there exists a unique solution* $z \in Z + z^D$ *to* $\mathcal{P}(z,u) = 0$. *Moreover, there is a constant* $c > 0$ *such that*

$$\|z - \widehat{z}\|_Z \le c\,\|u - \widehat{u}\|_Y \quad \forall u, \widehat{u} \in Y,\ \mathcal{P}(z,u) = \mathcal{P}(\widehat{z},\widehat{u}) = 0. \tag{3.1}$$

*Let* $S = [0,T]$, $T > 0$. *Then for every* $u \in L^2(S,Y)$ *there exists a unique* $z \in L^2(S,Z) + z^D$ *such that* $\mathcal{P}(z(t),u(t)) = 0$ *f.a.a.* $t \in S$. *If* $u \in C(S,Y)$, *then* $z \in C(S,Z) + z^D$ *follows and the last equation is fulfilled for all* $t \in S$.

*Proof.* The problem $\mathcal{P}(z,u) = 0$ may be written equivalently by $\mathcal{P}_0(z - z^D) = g(z^D,u)$ with $g(z^D,u)$ and the Lipschitz continuous and strongly monotone operator $\mathcal{P}_0\colon Z \to Z^*$,

$$\begin{aligned}\langle g(z^D,u),\widehat{y}\rangle_Z &= \int_\Omega \left\{ \left( f + \sum_{i=1}^{2} \lambda_i u_i \right) \widehat{y} - \varepsilon \nabla z^D \cdot \nabla \widehat{y} \right\} \mathrm{d}x \\ &\quad + \sum_{i=3}^{4} \int_G \lambda_i u_i \widehat{y}\,\mathrm{d}\mu + \sum_{i=1}^{2} \int_{G_\Gamma} \lambda_{\Gamma i} u_{\Gamma i} \widehat{y}\,\mathrm{d}\mu_\Gamma, \\ \langle \mathcal{P}_0 y, \widehat{y}\rangle_Z &= \int_\Omega \varepsilon \nabla y \cdot \nabla \widehat{y}\,\mathrm{d}x, \quad y,\, \widehat{y} \in Z.\end{aligned}$$

To show $g(z^D,u) \in Z^*$, for the last two terms we argue as follows: Because of assumption assumption (A2) we have for all $\widehat{y} \in Z$, and $i = 1,2$ the estimates

$$\int_G u_{i+2} \widehat{y}\,\mathrm{d}\mu \le c\|u_{i+2}\|_{L^2(G;\mathrm{d}\mu)} \|\widehat{y}\|_Z, \ \int_{G_\Gamma} u_{\Gamma i} \widehat{y}\,\mathrm{d}\mu_\Gamma \le c\|u_{\Gamma i}\|_{L^2(G_\Gamma;\mathrm{d}\mu_\Gamma)} \|\widehat{y}\|_Z.$$

Therefore, for all right-hand sides $g(z^D,u) \in Z^*$ there is a unique solution to $\mathcal{P}_0(z - z^D) = g(z^D,u)$ and (3.1) follows immediately. As a direct consequence we obtain the result for the time dependent functions. ∎

*Remark.* If $(u,z)$ is a solution to (P), then $u \in C(\mathbb{R}_+,Y)$. Thus, by Lemma 3.1 $z - z^D \in C(\mathbb{R}_+,Z)$ and for all $t \in \mathbb{R}_+$ the relations $\mathcal{P}(z(t),u(t)) = 0$ in $Z^*$, $u_i(t) \ge 0$ a.e. on $\Omega$, $i = 1,2$, $u_i(t) \ge 0$ $\mu$-a.e. on $G$, $i = 3,4$, $u_{\Gamma i}(t) \ge 0$, $\mu_\Gamma$-a.e. on $G_\Gamma$, $i = 1,2$, are fulfilled.

Lemma 3.2. (i) *We presume assumptions* (A1)–(A6). *If* $(u,z)$ *is a solution to* (P), *then for all* $t \in \mathbb{R}_+$,

$$\begin{aligned}&u_3(t) + u_4(t) = U_3 + U_4 = 1, \quad 0 \le u_3(t),\, u_4(t) \le 1 \quad \mu\text{-a.e. on } G,\\ &u_{\Gamma 1}(t) + u_{\Gamma 2}(t) = U_{\Gamma 1} + U_{\Gamma 2} = 1, \quad 0 \le u_{\Gamma 1}(t),\, u_{\Gamma 2}(t) \le 1 \quad \mu_\Gamma\text{-a.e. on } G_\Gamma.\end{aligned}$$

(ii) *We assume assumptions* (A1)–(A6). *Then there exist constants* $q > 2$ *and* $c > 0$ *such that*

$$\|z\|_{W^{1,q}} \le c \left\{ 1 + \sum_{i=1}^{2} \|u_i\|_{L^{2q/(2+q)}} \right\} \tag{3.2}$$

*for any solution* $(u,z)$ *to* (P).

*Proof.* (i) The result for $u_3$ and $u_4$ is obtained as in the proof of [9, Lemma 3.2]. By similar ideas, we test the ODEs for $u_{\Gamma 1}$ and $u_{\Gamma 2}$ by $\mu_\Gamma(B_\varrho^{G_\Gamma}(y))^{-1}\,\chi_{B_\varrho^{G_\Gamma}(y)}$ (where $B_\varrho^{G_\Gamma}(y)$ is the intersection of $G_\Gamma$ and the ball centered at $y$ with radius $\varrho$ and $\chi$ denotes the characteristic function) and let $\varrho \downarrow 0$ the assertions for $u_{\Gamma 1}$ and $u_{\Gamma 2}$ follow.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

(ii) We use the notation of the proof of Lemma 3.1. According to Gröger's regularity result for elliptic equations with nonsmooth data [13, Theorem 1] and assumptions (A4), (A1), we can fix a $q = q(\Omega, \varepsilon) > 2$ such that, if

$$\forall \widehat{y} \in H_0^1(\Omega \cup \Gamma_N): \ \langle \mathcal{P}_0 y, \widehat{y} \rangle_Z = \langle g, \widehat{y} \rangle, \quad g \in W^{-1,q}(\Omega \cup \Gamma_N),\ y \in H_0^1(\Omega \cup \Gamma_N),$$

then $y \in W_0^{1,q}(\Omega \cup \Gamma_N)$. We set

$$r = \frac{2q}{q-2}, \quad r' = \frac{2q}{q+2}, \quad s = \frac{q}{q-2}, \quad s' = \frac{q}{2}. \tag{3.3}$$

Note that $g(z^D, u) \in W^{-1,q}(\Omega \cup \Gamma_N)$. We again use assumption (A2) to estimate

$$\begin{aligned} &\int_G u_{i+2} \widehat{y}\, \mathrm{d}\mu \le c \|u_{i+2}\|_{L^{r'}(G;\mathrm{d}\mu)} \|\widehat{y}\|_{L^r} \le c \|u_{i+2}\|_{L^{r'}(G;\mathrm{d}\mu)} \|\widehat{y}\|_{W^{1,q'}}, \\ &\int_{G_\Gamma} u_{\Gamma i} \widehat{y}\, \mathrm{d}\mu_\Gamma \le c \|u_{\Gamma i}\|_{L^{s'}(G_\Gamma;\mathrm{d}\mu_\Gamma)} \|\widehat{y}\|_{L^s(\Gamma)} \le c \|u_{\Gamma i}\|_{L^{s'}(G_\Gamma;\mathrm{d}\mu_\Gamma)} \|\widehat{y}\|_{W^{1,q'}}, \quad i = 1, 2. \end{aligned}$$

Gröger's regularity result thus implies

$$\begin{aligned} \|z - z^D\|_{W_0^{1,q}} &\le c \|g(z^D, u)\|_{W^{-1,q}} \\ &\le c \left( 1 + \sum_{i=1}^2 \|u_i\|_{L^{r'}} + \sum_{i=3}^4 \|u_i\|_{L^{r'}(G;\mathrm{d}\mu)} + \sum_{i=1}^2 \|u_{\Gamma i}\|_{L^{s'}(G_\Gamma;\mathrm{d}\mu_\Gamma)} \right). \end{aligned}$$

Therefore, due to assumption (A4) and part (i) of Lemma 3.2 the desired estimate follows. ∎

LEMMA 3.3. *We presume assumptions* (A1)–(A6). *Then for all* $\tau > 0$ *there exist constants* $c_\tau > 0$, $c > 0$ *such that*

$$\begin{aligned} &\int_0^t \sum_{\gamma=\alpha,\beta} \left( \|r_{\Gamma 1}^\gamma u_1^\gamma u_{\Gamma 2}\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)} + \|r_{\Gamma 2}^\gamma u_2^\gamma u_{\Gamma 1}\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)} \right) \mathrm{d}s \\ &\quad + \sum_{i=1}^2 \int_0^t \left| \int_\Gamma \sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta \,\mathrm{d}a \right| \mathrm{d}s \\ &\le c + \int_0^t \left\{ c + \sum_{i=1}^2 \left\{ \tau \|2\nabla\sqrt{u_i} + \lambda_i \sqrt{u_i}\, \nabla z\|_{L^2(\Omega)}^2 + c_\tau \|u_i\|_{L^1(\Omega)} \right\} \right\} \mathrm{d}s \quad \forall t > 0 \end{aligned}$$

*for any solution* $(u, z)$ *to* (P).

*Proof.* Due to assumption (A1), for $\gamma = \alpha, \beta$ we find Lipschitz continuous functions $\phi^\gamma : \bar{\Omega}^\gamma \to [0, 1]$ with $\phi^\gamma = 0$ on $\Gamma_D^\gamma$, $\phi^\gamma = 1$ on $\Gamma$, and $|\nabla \phi^\gamma| \le 1/\kappa_0$. Testing the equations for $u_i$, $i = 1, 2$, on $\Omega^\alpha$ by $\phi^\alpha$, adding them, and having in mind Lemma 3.2 (i), assumptions (A4), (A5), (A6) we obtain

$$\begin{aligned} &\sum_{i=1}^2 \|u_i(t)\phi^\alpha\|_{L^1(\Omega^\alpha)} + \int_0^t \left\{ \int_{\Omega^\alpha} 2 r_0 u_1 u_2 \phi^\alpha \,\mathrm{d}x + \int_{\Omega^\alpha \times E_G} (r_1 u_1 u_4 + r_2 u_2 u_3) \phi^\alpha \mathrm{d}\mu \right\} \mathrm{d}s \\ &\quad + \int_0^t \left\{ \int_{G_\Gamma} (r_{\Gamma 1}^\alpha u_1^\alpha u_{\Gamma 2} + r_{\Gamma 2}^\alpha u_2^\alpha u_{\Gamma 1}) \,\mathrm{d}\mu_\Gamma + \sum_{i=1}^2 \int_\Gamma (\sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta) \,\mathrm{d}a \right\} \mathrm{d}s \\ &\le \sum_{i=1}^2 \left\{ \|U_i\|_{L^1(\Omega^\alpha)} + \int_0^t \left\{ c + \int_{\Omega^\alpha} \frac{D_i}{\kappa_0} |\nabla u_i + \lambda_i u_i \nabla z| \mathrm{d}x \right\} \mathrm{d}s \right\} \quad \forall t > 0. \end{aligned}$$

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

The terms in the first line can be left out since they are nonnegative. The last term in the last line can be estimated as follows where at the end Young's inequality is used,

$$\int_{\Omega^\alpha} \frac{D_i}{\kappa_0}|\nabla u_i + \lambda_i u_i \nabla z|\,\mathrm{d}x \le c\int_{\Omega^\alpha}\sqrt{u_i}|2\nabla\sqrt{u_i} + \lambda_i\sqrt{u_i}\,\nabla z|\,\mathrm{d}x \\ \le \tau\|2\nabla\sqrt{u_i} + \lambda_i\sqrt{u_i}\,\nabla z\|^2_{L^2(\Omega^\alpha)} + c_\tau\|u_i\|_{L^1(\Omega^\alpha)}.$$

Similar results are obtained by testing the equations for $u_i$, $i = 1, 2$, on $\Omega^\beta$ by $\phi^\beta$, only the term $\int_\Gamma(\sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta)\,\mathrm{d}a$ then has the opposite sign. Combining both estimates, the assertion of the follows. $\square$

Using $z^D$, $u_1^{\gamma D}$, $u_2^{\gamma D}$ and $\widetilde{u}_3$, $\widetilde{u}_4$, $\widetilde{u}_{\Gamma 1}$, $\widetilde{u}_{\Gamma 2}$ from (A5), we define the two functionals $\widetilde{F}_1, \widetilde{F}_2 \colon Y_+ \to \mathbb{R}$,

$$\widetilde{F}_1(u) := \int_\Omega \frac{\varepsilon}{2}|\nabla(z - z^D)|^2\,\mathrm{d}x,$$

$$\widetilde{F}_2(u) := \int_\Omega \sum_{i=1}^2 \left\{u_i\left(\ln\frac{u_i}{u_i^D} - 1\right) + u_i^D\right\}\mathrm{d}x + \sum_{i=3}^4\int_G\left\{u_i\ln\frac{u_i}{\widetilde{u}_i} - u_i + \widetilde{u}_i\right\}\mathrm{d}\mu \\ + \sum_{i=1}^2\int_{G_\Gamma}\left\{u_{\Gamma i}\ln\frac{u_{\Gamma i}}{\widetilde{u}_{\Gamma i}} - u_{\Gamma i} + \widetilde{u}_{\Gamma i}\right\}\mathrm{d}\mu_\Gamma,$$

where $z$ is the solution to $\mathcal{P}(z, u) = 0$ (see Lemma 3.1). The value $\widetilde{F}_1(u) + \widetilde{F}_2(u)$ can be interpreted as free energy of the state $u$. Because of assumption (A4) we find for $u \in Y_+$ the estimate

$$\|z - z^D\|_Z^2 + \sum_{i=1}^2\|u_i\ln u_i\|_{L^1} + \sum_{i=3}^4\|u_i\ln u_i\|_{L^1(G,\mathrm{d}\mu)} + \sum_{i=1}^2\|u_{\Gamma i}\ln u_{\Gamma i}\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)} \\ \le c\big(\widetilde{F}_1(u) + \widetilde{F}_2(u) + 1\big).$$

We extend $\widetilde{F}_k$, $k = 1, 2$, to arguments from the space $X^*$ by the definition

$$F_k := (\widetilde{F}_k^*|_X)^* \colon X^* \to \overline{\mathbb{R}}, \quad k = 1, 2.$$

The star denotes the conjugation (see [3]). Following the ideas in [9, subsection 3.4] we find that the free energy functional $F := F_1 + F_2$ is proper, convex, and lower semicontinuous. For $u \in Y_+$ the relation $F(u) = \widetilde{F}_1(u) + \widetilde{F}_2(u)$ is fulfilled, $F|_{Y_+}$ is continuous. Moreover, if $u \in Y_+$, $u > \delta$ and $(\ln\frac{u_1}{u_1^D}, \ln\frac{u_2}{u_2^D}, \ln\frac{u_3}{\widetilde{u}_3}, \ln\frac{u_4}{\widetilde{u}_4}, \ln\frac{u_{\Gamma 1}}{\widetilde{u}_{\Gamma 1}}, \ln\frac{u_{\Gamma 2}}{\widetilde{u}_{\Gamma 2}}) \in X$, then

$$\lambda(z - z^D) + \left(\ln\frac{u_1}{u_1^D}, \ln\frac{u_2}{u_2^D}, \ln\frac{u_3}{\widetilde{u}_3}, \ln\frac{u_4}{\widetilde{u}_4}, \ln\frac{u_{\Gamma 1}}{\widetilde{u}_{\Gamma 1}}, \ln\frac{u_{\Gamma 2}}{\widetilde{u}_{\Gamma 2}}\right) \in \partial F(u).$$

THEOREM 3.4. *We presume assumption* (A1)–(A6). *Let* $(u, z)$ *be a solution to* (P) *and* $T \in \mathbb{R}_+$. *Then*

$$F(u(t)) \le (F(U) + c_0)e^{c_0 t} \quad \forall t \in [0, T],$$

*where* $c_0 > 0$ *is a constant independent of* $U$ *and* $T$. *Moreover, if*

$$G_{phot} = 0,\ u_1^D u_2^D = k_0,\ \text{and}\ \ln u_i^{\gamma D} + \lambda_i z^D\ \textit{is constant on}\ \Omega^\gamma,\ \gamma = \alpha, \beta,\ i = 1, 2, \tag{3.4}$$

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

*and if*

(3.5) $$k_1k_2 = u_1^D u_2^D \ \mu\text{-a.e. on } G,\ \frac{k_{\Gamma 1}^{\alpha}}{k_{\Gamma 1}^{\beta}} = \frac{u_1^{\alpha D}}{u_1^{\beta D}},\ k_{\Gamma 1}^{\gamma}k_{\Gamma 2}^{\gamma} = u_1^{\gamma D}u_2^{\gamma D},\ \mu_\Gamma\text{-a.e. on } G_\Gamma,$$

*$\gamma = \alpha, \beta$, then $c_0$ can be chosen as zero.*

*Proof.* 1. We formally use the test function

$$\lambda(z - z^D) + \left(\ln\frac{u_1}{u_1^D}, \ln\frac{u_2}{u_2^D}, \ln\frac{u_3}{\widetilde{u}_3}, \ln\frac{u_4}{\widetilde{u}_4}, \ln\frac{u_{\Gamma 1}}{\widetilde{u}_{\Gamma 1}}, \ln\frac{u_{\Gamma 2}}{\widetilde{u}_{\Gamma 2}}\right)$$

for (P) and apply Brézis formula (see A.1 or [2, Lemma 3.3]). (To derive the desired result precisely, one has to use test functions

$$\lambda(z - z^D) + \left(\ln\frac{u_1^\delta}{u_1^D}, \ln\frac{u_2^\delta}{u_2^D}, \ln\frac{u_3^\delta}{\widetilde{u}_3}, \ln\frac{u_4^\delta}{\widetilde{u}_4}, \ln\frac{u_{\Gamma 1}^\delta}{\widetilde{u}_{\Gamma 1}}, \ln\frac{u_{\Gamma 2}^\delta}{\widetilde{u}_{\Gamma 2}}\right), \quad u^\delta = \max\{u, \delta\},$$

(3.6) $$0 < \delta < \min\left\{\min_{i=1,2}\{\operatorname*{ess\,inf}_{\Omega} U_i, \operatorname*{ess\,inf}_{\Omega} u_i^D\}, \min_{i=3,4}\{\operatorname*{ess\,inf}_{G,\mu} U_i\}, \min_{i=1,2}\{\operatorname*{ess\,inf}_{G_\Gamma,\mu_\Gamma} U_{\Gamma i}\}\right\},$$

and then one has to take the limit $\delta \downarrow 0$; see steps $1, 2$ in the proof of [9, Theorem 3.2].)

2. We estimate a.e. in $\Omega$ that

$$\begin{aligned}
D_i(\nabla u_i + \lambda_i u_i \nabla z) \cdot \nabla(\ln \tfrac{u_i}{u_i^D} + \lambda_i(z - z^D)) \qquad\qquad&\\
\geq \frac{\epsilon}{2}|2\nabla\sqrt{u_i} + \lambda_i\sqrt{u_i}\nabla z|^2 - cu_i|\nabla(\ln u_i^D + \lambda_i z^D)|^2&,\\
G_{phot}(\ln \tfrac{u_i}{u_i^D} + \lambda_i(z - z^D)) \leq |G_{phot}|(|u_i| + |\ln u_i^D| + |z - z^D|)&,\\
r_0(u_1u_2 - k_0)\ln\tfrac{u_1u_2}{u_1^Du_2^D} \geq -c|\ln\tfrac{u_1^Du_2^D}{k_0}|&.
\end{aligned}$$

The last line follows by a case by case analysis. Have in mind that all considered reactions are charge conserving. Moreover, we find by the monotonicity of the logarithm function and by $u_1^D\widetilde{u}_4 = k_1\widetilde{u}_3$ (see assumption (A5)) that $\mu$-a.e. on $G$

$$\begin{aligned}
r_1(u_1u_4 - k_1u_3)\ln\tfrac{u_1u_4\widetilde{u}_3}{u_1^D\widetilde{u}_4u_3} &= r_1(u_1u_4 - k_1u_3)\ln\tfrac{u_1u_4}{k_1u_3} \geq 0,\\
r_2(u_2u_3 - k_2u_4)\ln\tfrac{u_2u_3\widetilde{u}_4}{u_2^D\widetilde{u}_3u_4} &= r_2(u_2u_3 - k_2u_4)\Big[\ln\tfrac{u_2u_3}{k_2u_4} + \ln\tfrac{k_1k_2}{u_1^Du_2^D}\Big]\\
&\geq -c(|u_2| + 1)|\ln\tfrac{k_1k_2}{u_1^Du_2^D}|.
\end{aligned}$$

Additionally, using that $u_1^{\alpha D}\widetilde{u}_{\Gamma 2} = k_{\gamma 1}^{\alpha}\widetilde{u}_{\Gamma 1}$ (see assumption (A5)) we establish that $\mu_\Gamma$-a.e. on $G_\Gamma$

$$\begin{aligned}
r_{\Gamma 1}^{\alpha}(u_1^{\alpha}u_{\Gamma 2} - k_{\Gamma 1}^{\alpha}u_{\Gamma 1})\ln\tfrac{u_1^{\alpha}u_{\Gamma 2}\widetilde{u}_{\Gamma 1}}{u_1^{\alpha D}\widetilde{u}_{\Gamma 2}u_{\Gamma 1}} &= r_{\Gamma 1}^{\alpha}(u_1^{\alpha}u_{\Gamma 2} - k_{\Gamma 1}^{\alpha}u_{\Gamma 1})\ln\tfrac{u_1^{\alpha}u_{\Gamma 2}}{k_{\Gamma 1}^{\alpha}u_{\Gamma 1}} \geq 0,\\
r_{\Gamma 1}^{\beta}(u_1^{\beta}u_{\Gamma 2} - k_{\Gamma 1}^{\beta}u_{\Gamma 1})\ln\tfrac{u_1^{\beta}u_{\Gamma 2}\widetilde{u}_{\Gamma 1}}{u_1^{\beta D}\widetilde{u}_{\Gamma 2}u_{\Gamma 1}} &= r_{\Gamma 1}^{\beta}(u_1^{\beta}u_{\Gamma 2} - k_{\Gamma 1}^{\beta}u_{\Gamma 1})\Big[\ln\tfrac{u_1^{\beta}u_{\Gamma 2}}{k_{\Gamma 1}^{\beta}u_{\Gamma 1}} + \ln\tfrac{k_{\Gamma 1}^{\beta}u_1^{\alpha D}}{k_{\Gamma 1}^{\alpha}u_1^{\beta D}}\Big]\\
&\geq -(r_{\Gamma 1}^{\beta}u_1^{\beta}u_{\Gamma 2} + c)|\ln\tfrac{k_{\Gamma 1}^{\beta}u_1^{\alpha D}}{k_{\Gamma 1}^{\alpha}u_1^{\beta D}}|,\\
r_{\Gamma 2}^{\alpha}(u_2^{\alpha}u_{\Gamma 1} - k_{\Gamma 2}^{\alpha}u_{\Gamma 2})\ln\tfrac{u_2^{\alpha}u_{\Gamma 1}\widetilde{u}_{\Gamma 2}}{u_2^{\alpha D}\widetilde{u}_{\Gamma 1}u_{\Gamma 2}} &= r_{\Gamma 2}^{\alpha}(u_2^{\alpha}u_{\Gamma 1} - k_{\Gamma 2}^{\alpha}u_{\Gamma 2})\Big[\ln\tfrac{u_2^{\alpha}u_{\Gamma 1}}{k_{\Gamma 2}^{\alpha}u_{\Gamma 2}} + \ln\tfrac{k_{\Gamma 1}^{\alpha}k_{\Gamma 2}^{\alpha}}{u_1^{\alpha D}u_2^{\alpha D}}\Big]\\
&\geq -(r_{\Gamma 2}^{\alpha}u_2^{\alpha}u_{\Gamma 1} + c)|\ln\tfrac{k_{\Gamma 1}^{\alpha}k_{\Gamma 2}^{\alpha}}{u_1^{\alpha D}u_2^{\alpha D}}|,\\
r_{\Gamma 2}^{\beta}(u_2^{\beta}u_{\Gamma 1} - k_{\Gamma 2}^{\beta}u_{\Gamma 2})\ln\tfrac{u_2^{\beta}u_{\Gamma 1}\widetilde{u}_{\Gamma 2}}{u_2^{\beta D}\widetilde{u}_{\Gamma 1}u_{\Gamma 2}} &= r_{\Gamma 2}^{\beta}(u_2^{\beta}u_{\Gamma 1} - k_{\Gamma 2}^{\beta}u_{\Gamma 2})\Big[\ln\tfrac{u_2^{\beta}u_{\Gamma 1}}{k_{\Gamma 2}^{\beta}u_{\Gamma 2}} + \ln\tfrac{k_{\Gamma 1}^{\alpha}k_{\Gamma 2}^{\beta}}{u_1^{\alpha D}u_2^{\beta D}}\Big]\\
&\geq -(r_{\Gamma 2}^{\beta}u_2^{\beta}u_{\Gamma 1} + c)|\ln\tfrac{k_{\Gamma 1}^{\alpha}k_{\Gamma 2}^{\beta}}{u_1^{\alpha D}u_2^{\beta D}}|,
\end{aligned}$$

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

and by $u_i^{\gamma D}|_\Gamma = \frac{1}{\sigma_i^\gamma}$ $i=1,2$, $\gamma=\alpha,\beta$, (see assumption (A5)) we conclude that

$$(\sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta)\ln\frac{u_i^\alpha u_i^{\beta D}}{u_i^{\alpha D}u_i^\beta} = (\sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta)\ln\frac{\sigma_i^\alpha u_i^\alpha}{\sigma_i^\beta u_i^\beta} = 0 \qquad \text{a.e. on } \Gamma, \quad i=1,2.$$

According to our assumptions (A3), (A4), and (A5), we find from step 1 and the previous estimates

$$\begin{aligned}
&F(u(t)) - F(U) + \frac{\epsilon}{2}\int_0^t \|2\nabla\sqrt{u_i} + \lambda_i\sqrt{u_i}\,\nabla z\|_{L^2}^2\,\mathrm{d}s\\
&\le c\int_0^t \sum_{i=1}^2 (1+\|u_i\|_{L^1})\Big(\|\nabla(\ln u_i^D + \lambda_i z^D)\|_{L^\infty}^2 + \|\ln\tfrac{u_1^D u_2^D}{k_0}\|_{L^\infty} + \|\ln\tfrac{k_1k_2}{u_1^D u_2^D}\|_{L^\infty(G,\mathrm{d}\mu)}\Big)\,\mathrm{d}s\\
&\quad + c\int_0^t (1+\|r_{\Gamma 1}^\beta u_1^\beta u_{\Gamma 2}\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)})\|\ln\tfrac{k_{\Gamma 1}^\beta u_1^{\alpha D}}{k_{\Gamma 1}^\alpha u_1^{\beta D}}\|_{L^\infty(G_\Gamma,\mathrm{d}\mu_\Gamma)}\,\mathrm{d}s\\
&\quad + c\int_0^t (1+\|r_{\Gamma 2}^\alpha u_2^\alpha u_{\Gamma 1}\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)})\|\ln\tfrac{k_{\Gamma 1}^\alpha k_{\Gamma 2}^\alpha}{u_1^{\alpha D}u_2^{\alpha D}}\|_{L^\infty(G_\Gamma,\mathrm{d}\mu_\Gamma)}\,\mathrm{d}s\\
&\quad + c\int_0^t (1+\|r_{\Gamma 2}^\beta u_2^\beta u_{\Gamma 1}\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)})\|\ln\tfrac{k_{\Gamma 1}^\alpha k_{\Gamma 2}^\beta}{u_1^{\alpha D}u_2^{\beta D}}\|_{L^\infty(G_\Gamma,\mathrm{d}\mu_\Gamma)}\,\mathrm{d}s\\
&\quad + \int_0^t \|G_{phot}\|_{L^\infty}\left\{\sum_{i=1}^2\big(\|u_i\|_{L^1} + \|\ln u_i^D\|_{L^1}\big) + \|z - z^D\|_{L^1}\right\}\mathrm{d}s.
\end{aligned}$$

3. If (3.4) and (3.5) are fulfilled, then the right-hand side of the previous estimate is zero. Therefore, the last assertion of Theorem 3.4 follows immediately. For the more general situation we argue as follows: Using assumption (A3), (A4), (A5), and Lemma 3.3 the right-hand side in the previous estimate can be majorized by

$$\int_0^t \sum_{i=1}^2 \Big(c\big(\|u_i\|_{L^1} + \|z - z^D\|_Z^2 + 1\big) + \frac{\epsilon}{2}\|2\nabla\sqrt{u_i} + \lambda_i\sqrt{u_i}\,\nabla z\|_{L^2}^2\Big)\,\mathrm{d}s.$$

Since $\sum_{i=1}^2 \|u_i\|_{L^1} + \|z-z^D\|_Z^2 \le cF(u) + c$ for $z$ with $\mathcal{P}(z,u)=0$, Gronwall's lemma supplies the desired result. □

*Remark.* Theorem 3.4 guarantees that the electronic model for solar cells including interface kinetics and energy resolved defect densities in $\Omega$ and at the interface $\Gamma$ is thermodynamically correct. The free energy functional $F$ is something like a Lyapunov function. Namely, under the special assumptions (3.4) and (3.5) (meaning that the data is compatible with thermodynamic equilibrium) the function $t \mapsto F(u(t))$ is monotonously decreasing. For the more general case of data the free energy may be increasing, but its growth can be estimated by Theorem 3.4.

*Remark.* If $r_0$ is independent of $u_1$, $u_2$ and $G_{phot}$ is independent of time, and the Dirichlet values and reaction constants fulfill

$$u_1^D u_2^D = k_0 + \frac{G_{phot}}{r_0},\ \ln u_i^{\gamma D} + \lambda_i z^D \text{ is constant on } \Omega^\gamma,\ \gamma=\alpha,\beta,\ i=1,2, \tag{3.7}$$

instead of (3.4) in Theorem 3.4 and if additionally (3.5) holds true, then the free energy on solutions $F(u(t))$ decreases monotonously, too. This can be seen by substituting the second and third estimate in step 2 of the proof of Theorem 3.4 by

$$r_0\Big(u_1u_2 - k_0 - \frac{G_{phot}}{r_0}\Big)\ln\frac{u_1u_2}{u_1^D u_2^D} \ge -\left|\ln\frac{u_1^D u_2^D}{k_0 + \frac{G_{phot}}{r_0}}\right|,$$

which is obtained by a case-by-case analysis, too.

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

**3.2. $L^\infty$-estimates of the solution.** Have in mind that Lemma 3.2 provides global upper and lower bounds for $u_3$, $u_4$ on $G$ and $u_{\Gamma1}$, $u_{\Gamma2}$ on $G_\Gamma$. To prove upper bounds for the densities of electrons and holes we argue in two steps. Starting with estimates of the $L^\infty(\mathbb{R}_+, L^2)$-norm of $u_i$, $i = 1, 2$, (see Lemma 3.5) the final estimate is obtained by Moser iteration in Theorem 3.6.

LEMMA 3.5. *Under the assumptions* (A1)–(A6) *there exists a monotonous function $d : \mathbb{R}_+ \to \mathbb{R}_+$ depending only on the data* (*but not on $T$*) *such that*

$$\sum_{i=1}^{2} \|u_i(t)\|_{L^2} \le d(\|F(u)\|_{C(S)}) \quad \forall t \in S = [0, T]$$

*for any solution* $(u, z)$ *to* (P).

*Proof.* For problem (P) we use the test function $\mathrm{e}^{2t}(v_1, v_2, 0, \dots, 0)$,

$$(3.8)\quad v_i := (u_i - K)^+, \quad \text{where } K \ge \hat{K} := \max\left(1, \|U\|_V, \max_{i=1,2,\ \gamma=\alpha,\beta} \|u_i^{\gamma D}\|_{L^\infty(\Omega^\gamma)}\right)$$

will be fixed later. The choice of $\hat{K}$ ensures that $v_i^\gamma(0) = 0$, $v_i^\gamma|_{\Gamma_D^\gamma} = 0$, $\gamma = \alpha, \beta$, $i = 1, 2$,

$$\begin{aligned}
&\frac{\mathrm{e}^{2t}}{2} \sum_{i=1}^{2} \int_\Omega v_i(t)^2 \,\mathrm{d}x \\
&= \int_0^t \mathrm{e}^{2s} \Bigg\{ \int_\Omega \sum_{i=1}^{2} \left\{ v_i^2 - D_i(\nabla v_i + \lambda_i u_i \nabla z) \cdot \nabla v_i + G_{phot} v_i + r_0(k_0 - u_1 u_2) v_i \right\} \mathrm{d}x \\
&\qquad + \sum_{i=1}^{2} \int_\Gamma (\sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta)(v_i^\beta - v_i^\alpha) \,\mathrm{d}a \\
&\qquad + \int_G \left\{ r_1(k_1 u_3 - u_1 u_4) v_1 + r_2(k_2 u_4 - u_2 u_3) v_2 \right\} \mathrm{d}\mu \\
&\qquad + \sum_{\gamma=\alpha,\beta} \int_{G_\Gamma} \left\{ r_{\Gamma1}^\gamma (k_{\Gamma1}^\gamma u_{\Gamma1} - u_1^\gamma u_{\Gamma2}) v_1^\gamma + r_{\Gamma2}^\gamma (k_{\Gamma2}^\gamma u_{\Gamma2} - u_2^\gamma u_{\Gamma1}) v_2^\gamma \right\} \mathrm{d}\mu_\Gamma \Bigg\} \mathrm{d}s \\
&\le \int_0^t \mathrm{e}^{2s} \sum_{i=1}^{2} \Bigg\{ -\epsilon \|v_i\|_{H^1}^2 + c\|u_i\|_{L^r} \|\nabla z\|_{L^q} \|v_i\|_{H^1} \\
&\qquad\qquad + c\|v_i\|_{L^2}^2 + c \sum_{\gamma=\alpha,\beta} \|v_i^\gamma\|_{L^2(\Gamma)}^2 + cK^2 \Bigg\} \mathrm{d}s.
\end{aligned}$$

The exponents $q > 2$ and $r$ are taken from Lemma 3.2 (ii) and (3.3). For the treatment of the reaction terms we refer to assumption (A3) and Lemma 3.2 (i). Moreover, due to assumption(A2) we have $\|v_i\|_{L^2(G,\mathrm{d}\mu)} \le c\|v_i\|_{L^2(\Omega)}$, $\|v_i^\gamma\|_{L^2(G_\Gamma,\mathrm{d}\mu_\Gamma)} \le c\|v_i^\gamma\|_{L^2(\Gamma)}$, $i = 1, 2$. Now we apply, the trace inequality (A.1), the estimate (3.2), and the three variants of the Gagliardo–Nirenberg inequality (A.2),

$$\|v_i\|_{L^2}^2 \le c\|v_i\|_{L^1} \|v_i\|_{H^1}, \quad \|v_i\|_{L^r} \le c\|v_i\|_{L^1}^{1/r} \|v_i\|_{H^1}^{1/r'}, \quad \|v_i\|_{L^{r'}} \le c\|v_i\|_{L^1}^{1/r'} \|v_i\|_{H^1}^{1/r}$$

with $r$ and $r'$ from (3.3). At the end, Young's inequality gives

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

(3.9)
$$\frac{e^{2t}}{2}\sum_{i=1}^{2}\|v_i(t)\|_{L^2}^2 \le \int_0^t \mathrm{e}^{2s}\sum_{i=1}^{2}\left\{\left(\tilde c\sum_{j=1}^{2}\|v_j\|_{L^1}-\frac{\epsilon}{2}\right)\|v_i\|_{H^1}^2+c(K)\big(\|v_i\|_{L^1}^2+1\big)\right\}\mathrm{d}s \quad \forall\, t\in S$$

with a monotonously increasing function $c(K)$. For $K$ fulfilling the inequality $\ln K > \max_{i=1,2,\,\gamma=\alpha,\beta}\|\ln u_i^{\gamma D}\|_{L^\infty(\Omega^\gamma)}+1$ we estimate

$$\begin{aligned}F(u) &\ge \sum_{i=1}^{2}\int_\Omega\left\{u_i\left(\ln\tfrac{u_i}{u_i^D}-1\right)+u_i^D\right\}\mathrm{d}x\\ &\ge \sum_{i=1}^{2}\int_{\{x:v_i>0\}}u_i\left(\ln K-\max_{k=1,2,\,\gamma=\alpha,\beta}\|\ln u_k^{\gamma D}\|_{L^\infty(\Omega^\gamma)}-1\right)\mathrm{d}x\\ &\ge \left(\ln K-\max_{k=1,2,\,\gamma=\alpha,\beta}\|\ln u_k^{\gamma D}\|_{L^\infty(\Omega^\gamma)}-1\right)\sum_{i=1}^{2}\|v_i\|_{L^1}.\end{aligned}$$

Now we fix $K\ge\hat K$ as a monotonously increasing function of $\|F(u)\|_{C(S)}$ fulfilling

$$\tilde c\sum_{i=1}^{2}\|v_i\|_{L^1}\le \frac{\tilde c\|F(u)\|_{C(S)}}{\ln K-\max_{k=1,2,\,\gamma=\alpha,\beta}\|\ln u_k^{\gamma D}\|_{L^\infty(\Omega^\gamma)}-1}<\frac{\epsilon}{2}$$

(compare Theorem 3.4); then the term in front of the $H^1$-norm in (3.9) is negative. It results in

$$\mathrm{e}^{2t}\sum_{i=1}^{2}\|v_i(t)\|_{L^2}^2\le \mathrm{e}^{2t}\,c\,c(K)(\|F(u)\|_{C(S)}^2+1).$$

Since $u_i\le v_i+K$, this proves Lemma 3.5 $\square$

Lemmas 3.2, and 3.5 guarantee that for solutions $(u,z)$ to (P) for all $t\in S$ the norm $\|z(t)\|_{W^{1,q}(\Omega)}$ is bounded by a continuous function of $\|F(u)\|_{C(S)}$ depending on the data but not on $T$. The exponent $q>2$ results from Lemma 3.2 (ii). We write shortly

$$\kappa=\Big(\|\nabla z\|_{L^\infty(S,L^q(\Omega))}+1\Big)^{2r}. \tag{3.10}$$

Now we establish the upper bounds for the densities of electrons and holes. The proof is based on Moser iteration techniques. Such techniques, e.g., are used in [10] for problems from semiconductor technology, in [6] for the classical van Roosbroeck system and in [8] for spin-polarized drift-diffusion systems.

THEOREM 3.6. *Let assumptions* (A1)–(A6) *be satisfied. Then there exists a constant $c>0$ and a continuous function $d$ of $\|F(u)\|_{C(S)}$ depending only on the data* (*but not on $T$*) *such that*

$$\sum_{i=1}^{2}\|u_i(t)\|_{L^\infty}\le c\,\kappa\sum_{i=1}^{2}\left(\sup_{s\in S}\|u_i(s)\|_{L^1}+1\right),\qquad \|z(t)\|_{L^\infty}\le d(\|F(u)\|_{C(S)})\quad \forall t\in S$$

*for any solution $(u,z)$ to* (P).

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Note that $\sup_{s\in S}\|u_i(s)\|_{L^1} \le c\,(\|F(u)\|_{C(S)}+1)$, $i=1,2$, on solutions to (P) and that this right-hand side is bounded by Theorem 3.4.

*Proof.* Using for (P) the test functions

$$p\,\mathrm{e}^{pt}\,(v_1^{p-1}, v_2^{p-1}, 0,\dots,0) \in L^2(S,X),\ p=2^m,\ m\ge 1,\ v_i := (u_i-\widehat{K})^+,\ i=1,2,$$

with $\widehat{K}$ from (3.8) we obtain

$$\begin{aligned}
&\mathrm{e}^{pt}\sum_{i=1}^2\int_\Omega v_i(t)^p\,\mathrm{d}x\\
&= \int_0^t p\mathrm{e}^{2s}\bigg\{\int_\Omega\sum_{i=1}^2\big\{v_i^p - D_i(\nabla v_i+\lambda_i u_i\nabla z)\cdot\nabla v_i^{p-1} + G_{phot}v_i^{p-1}\big\}\,\mathrm{d}x\\
&\quad+\int_\Omega\sum_{i=1}^2 r_0(k_0-u_1u_2)v_i^{p-1}\,\mathrm{d}x + \sum_{i=1}^2\int_\Gamma(\sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta)\big((v_i^\beta)^{p-1}-(v_i^\alpha)^{p-1}\big)\,\mathrm{d}a\\
&\quad+\sum_{\gamma=\alpha,\beta}\int_{G_\Gamma}\{r_{\Gamma1}^\gamma(k_{\Gamma1}^\gamma u_{\Gamma1}-u_1^\gamma u_{\Gamma2})(v_1^\gamma)^{p-1} + r_{\Gamma2}^\gamma(k_{\Gamma2}^\gamma u_{\Gamma2}-u_2^\gamma u_{\Gamma1})(v_2^\gamma)^{p-1}\}\,\mathrm{d}\mu_\Gamma\\
&\quad+\int_G\{r_1(k_1u_3-u_1u_4)v_1^{p-1}+r_2(k_2u_4-u_2u_3)v_2^{p-1}\}\,\mathrm{d}\mu\bigg\}\,\mathrm{d}s\qquad\forall t\in S.
\end{aligned}$$

Regarding assumptions (A3), (A4), (A2), and Lemma 3.2, applying the trace inequality (A.1) for $(v_i^\gamma)^{p/2}$, and Hölder's, Gagliardo–Nirenberg's, and Young's inequality, we continue by

$$\begin{aligned}
\mathrm{e}^{pt}\sum_{i=1}^2\|v_i(t)\|_{L^p}^p &\le \int_0^t \mathrm{e}^{ps}\Big\{\int_\Omega\sum_{i=1}^2\Big\{cp\Big(u_i|\nabla z||\nabla v_i^{p-1}| + v_i^p + \Big(\sum_{k=1}^2 u_k+1\Big)v_i^{p-1}\Big)\Big\}\,\mathrm{d}x\\
&\qquad-\int_\Omega\sum_{i=1}^2\epsilon|\nabla v_i^{p/2}|^2\,\mathrm{d}x + cp\sum_{i=1}^2\sum_{\gamma=\alpha,\beta}\int_\Gamma\big((v_i^\gamma)^p+1\big)\,\mathrm{d}\Gamma\Big\}\,\mathrm{d}s\\
&\le\int_0^t\mathrm{e}^{ps}\sum_{i=1}^2\Big\{cp(\|\nabla z\|_{L^q}\|v_i^{p/2}\|_{L^r}+1)(\|v_i^{p/2}\|_{H^1}-\epsilon\|v_i^{p/2}\|_{H^1}^2)\\
&\qquad+cp\Big(\|v_i^{p/2}\|_{L^2}^2+\sum_{\gamma=\alpha,\beta}\|(v_i^\gamma)^{p/2}\|_{L^2(\Gamma)}^2+1\Big)\Big\}\,\mathrm{d}s\\
&\le\int_0^t\mathrm{e}^{ps}\Big\{\kappa\,c\,p^{2r}\sum_{i=1}^2(\|v_i^{p/2}\|_{L^1}^2+1)\,\mathrm{d}s\Big\},
\end{aligned}$$

where $\kappa$ is defined in (3.10). In summary it results the estimate

$$\sum_{i=1}^2\|v_i(t)\|_{L^p}^p \le cp^{2r}\kappa\sum_{i=1}^2\sup_{s\in S}(\|v_i(s)\|_{L^{p/2}}^p+1)\qquad\forall t\in S. \tag{3.11}$$

Defining

$$b_m=\sum_{i=1}^2\Big\{\sup_{s\in S}\|v_i(s)\|_{L^{2^m}}^{2^m}+1\Big\},\quad m=0,1,\dots$$

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

the inequality (3.11) implies

$$b_m \leq c^m \kappa\, b_{m-1}^2 \leq c^{m+2(m-1)} \kappa^{1+2} b_{m-2}^4 \leq \dots \leq c^{2^{m+1}-2-m} \kappa^{2^m-1} b_0^{2^m},$$

and we continue estimate (3.11) by

$$\sum_{i=1}^2 \|v_i(t)\|_{L^{2^m}} \leq c\kappa \sum_{i=1}^2 \Big\{ \sup_{s\in S} \|v_i(s)\|_{L^1} + 1 \Big\}.$$

In the limit $m \to \infty$, we find

$$\sum_{i=1}^2 \|v_i(t)\|_{L^\infty} \leq c\kappa \sum_{i=1}^2 \Big\{ \sup_{s\in S} \|v_i(s)\|_{L^1} + 1 \Big\} \qquad \forall t \in S.$$

Because of $u_i \leq v_i + \hat{K}$ the desired estimate for $u_i$, $i = 1, 2$, follows and then the assertion for $z$ is a direct consequence of Lemma 3.2 (ii) and the Sobolev embedding $W^{1,q}(\Omega) \hookrightarrow L^\infty(\Omega)$ for $q > 2$ in two spatial dimensions. ∎

## 4. Existence and uniqueness result for (P).

**4.1. A regularized problem ($\mathbf{P}_M$).** In order to show the existence of solutions to (P) we study a regularized problem ($\mathrm{P}_M$) defined on an arbitrarily fixed time interval $S = [0, T]$. For $M \geq M^* := \max\{1, \|U\|_V\}$ let $\rho_M : \mathbb{R}^6 \to [0, 1]$ be a Lipschitz continuous function fulfilling

$$\rho_M(u) = \begin{cases} 0 & \text{if } |u|_\infty \geq M, \\ 1 & \text{if } |u|_\infty \leq M/2, \end{cases} \qquad |u|_\infty = \max\{|u_1|, \dots, |u_{\Gamma 2}|\}.$$

Additionally, we introduce the projection

$$\sigma_M(y) := \begin{cases} -M & \text{for} \quad y < -M, \\ y & \text{for} \quad y \in [-M, M], \\ M & \text{for} \quad y > M, \end{cases} \qquad y \in \mathbb{R},$$

and define the operators $\mathcal{A}_M \colon (X + u^D) \times (Z + z^D) \to X^*$, $\mathcal{R}_M \colon [X + u^D] \cap V_+ \to X^*$,

$$\begin{aligned}
\langle \mathcal{A}_M(u, z), \widehat{u} \rangle_X &:= \int_\Omega \sum_{i=1}^2 D_i(\nabla u_i + \lambda_i [\sigma_M(u_i)]^+ \nabla z) \cdot \nabla \widehat{u}_i \,\mathrm{d}x, \\
\langle \mathcal{R}_M(u), \widehat{u} \rangle_X &:= \int_\Omega \rho_M(u) \Big\{ r_0(u_1 u_2 - k_0)(\widehat{u}_1 + \widehat{u}_2) - G_{phot}(\widehat{u}_1 + \widehat{u}_2) \Big\} \,\mathrm{d}x \\
&\quad + \int_G \rho_M(u) \Big\{ r_1(u_1 u_4 - k_1 u_3)(\widehat{u}_1 + \widehat{u}_4 - \widehat{u}_3) \\
&\qquad\qquad + r_2(u_2 u_3 - k_2 u_4)(\widehat{u}_2 + \widehat{u}_3 - \widehat{u}_4) \Big\} \,\mathrm{d}\mu \\
&\quad + \sum_{\gamma=\alpha,\beta} \int_{G_\Gamma} \rho_M(u) \Big\{ r_{\Gamma 1}^\gamma (u_1^\gamma u_{\Gamma 2} - k_{\Gamma 1}^\gamma u_{\Gamma 1})(\widehat{u}_1^\gamma + \widehat{u}_{\Gamma 2} - \widehat{u}_{\Gamma 1}) \\
&\qquad\qquad + r_{\Gamma 2}^\gamma (u_2^\gamma u_{\Gamma 1} - k_{\Gamma 2}^\gamma u_{\Gamma 2})(\widehat{u}_2^\gamma + \widehat{u}_{\Gamma 1} - \widehat{u}_{\Gamma 2}) \Big\} \,\mathrm{d}\mu_\Gamma \\
&\quad + \sum_{i=1}^2 \int_\Gamma \rho_M(u)(\sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta)(\widehat{u}_i^\alpha - \widehat{u}_i^\beta) \,\mathrm{d}a, \quad \widehat{u} \in X.
\end{aligned}$$

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

We study the regularized problem

$$(\mathrm{P}_M)\quad \begin{cases} u'(t)+\mathcal{A}_M(u(t),z(t))+\mathcal{R}_M(u^+(t))=0 \quad \mathcal{P}(z(t),u^+(t))=0, \quad \text{f.a.a. } t\in S,\\ u(0)=U,\ u\in H^1(S,X^*),\ u-u^D\in L^2(S,X),\ z-z^D\in L^2(S,Z). \end{cases}$$

Solutions $(u,z)$ to $(\mathrm{P}_M)$ fulfill $u\in C(S,Y)$ and $z-z^D\in C(S,Z)$.

**4.2. Solvability of $(\mathbf{P}_M)$.** In this subsection the constants may depend on $M$, and $S$. We work with an equivalent formulation of $(\mathrm{P}_M)$. We decompose $u$ in the form $u=(v,w)$, where $v=(u_1,u_2)$, $w=(u_3,u_4,u_{\Gamma 1},u_{\Gamma 2})$, and make use of the spaces

$$Y^2=L^2(\Omega)^2,\quad Y^4=L^2(G;\mathrm{d}\mu)^2\times L^2(G_\Gamma;\mathrm{d}\mu_\Gamma)^2,$$
$$X^2=(H^1(\Omega_N^\alpha)\times H^1(\Omega_N^\beta))^2,\quad X^{2*}:=(X^2)^*,$$

where $H^1(\Omega_N^\gamma):=H_0^1(\Omega\cup\Gamma_N^\gamma)$. We define operators $\mathcal{A}_v^0: L^2(S,X^2)\to L^2(S,X^{2*})$, $\mathcal{A}_v\colon (L^2(S,X^2)+v^D)\times(L^2(S,Z)+z^D)\to L^2(S,X^{2*})$, $\mathcal{R}_v\colon (L^2(S,X^2)+v^D)\times L^2(S,Y^4)\to L^2(S,X^{2*})$, and $\mathcal{R}_w\colon (L^2(S,X^2)+v^D)\times L^2(S,Y^4)\to L^2(S,Y^4)$ by

$$\langle\mathcal{A}_v^0(v-v^D),\widehat{v}\rangle_{L^2(S,X^2)}:=\int_S\int_\Omega\sum_{i=1}^2 D_i\nabla(v_i-v_i^D)\cdot\nabla\widehat{v}_i\,\mathrm{d}x\,\mathrm{d}s,$$

$$\langle\mathcal{A}_v(v,z),\widehat{v}\rangle_{L^2(S,X^2)}:=\int_S\int_\Omega\sum_{i=1}^2 D_i(\nabla v_i^D+\lambda_i\,[\sigma_M(v_i)]^+\nabla z)\cdot\nabla\widehat{v}_i\,\mathrm{d}x\,\mathrm{d}s,$$

$$\langle\mathcal{R}_v(v,w),\widehat{v}\rangle_{L^2(S,X^2)}:=\int_S\langle\mathcal{R}_M(v^+,w^+),(\widehat{v},0)\rangle_X\,\mathrm{d}s,\quad \widehat{v}\in L^2(S,X^2),$$

$$\langle\mathcal{R}_w(v,w),\widehat{w}\rangle_{L^2(S,Y^4)}:=\int_S\langle\mathcal{R}_M(v^+,w^+),(0,\widehat{w})\rangle_X\,\mathrm{d}s,\quad \widehat{w}\in L^2(S,Y^4).$$

Let $v\in L^2(S,Y^2)$ and $w\in L^2(S,Y^4)$. Then $(v,w)\in L^2(S,Y)$ and by Lemma 3.1 there is a unique solution $z$ with $z-z^D\in L^2(S,Z)\cap L^\infty(S,L^\infty(\Omega))$ of

$$\mathcal{P}(z(t),v^+(t),w^+(t))=0\quad \text{f.a.a. } t\in S.$$

By $\mathcal{T}_z\colon L^2(S,Y^2)\times L^2(S,Y^4)\to L^2(S,Z)+z^D$ we denote the corresponding solution operator such that $z=\mathcal{T}_z(v,w)$. Then the system

$$\begin{aligned}&(v-v^D)'+\mathcal{A}_v^0(v-v^D)=-\mathcal{R}_v(v,w)-\mathcal{A}_v(v,\mathcal{T}_z(v,w)),\\&(v-v^D)(0)=(U_1,U_2)-v^D,\quad v-v^D\in W^2,\end{aligned}\tag{4.1}$$

$$w'+\mathcal{R}_w(v,w)=0,\quad w(0)=(U_3,U_4,U_{\Gamma 1},U_{\Gamma 2}),\quad w\in H^1(S,Y^4),\tag{4.2}$$

is an equivalent formulation of problem $(\mathrm{P}_M)$. Note that here

$$W^2:=\{v\in L^2(S,X^2)\colon v'\in L^2(S,X^{2*})\}\subset C(S,Y^2).$$

Solvability of $(\mathrm{P}_M)$ is obtained by proving that the system (4.1), (4.2) has a solution. First, we give a short overview of this proof. For an arbitrarily fixed $\widehat{v}\in W^2+v^D$ we solve

$$w'+\mathcal{R}_w(\widehat{v},w)=0,\quad w(0)=(U_3,U_4,U_{\Gamma 1},U_{\Gamma 2}),\quad w\in H^1(S,Y^4),\tag{4.3}$$

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

and get $w = \mathcal{T}_w\widehat{v}$ with a solution operator $\mathcal{T}_w\colon W^2{+}v^D \to H^1(S, Y^4)$ (see Lemma 4.1). The problem

$$(4.4)\qquad \begin{aligned}(v - v^D)' + \mathcal{A}_v^0(v - v^D) &= -\mathcal{R}_v(\widehat{v}, \mathcal{T}_w\widehat{v}) - \mathcal{A}_v(\widehat{v}, \mathcal{T}_z(\widehat{v}, \mathcal{T}_w\widehat{v})),\\ (v - v^D)(0) &= (U_1, U_2) - v^D, \quad v - v^D \in W^2\end{aligned}$$

consists of four independent linear parabolic problems for $u_1^\alpha$, $u_1^\beta$, $u_2^\alpha$, $u_2^\beta$ and fixed given right-hand sides from $L^2(S, H^1(\Omega_N^\gamma))^*$. Thus there exists a unique solution $v = \mathcal{Q}\widehat{v}$ to this problem. The operator $\mathcal{Q}$ is completely continuous (see Lemma 4.2). Using Schauder's fixed point theorem we obtain a fixed point $v$ of $\mathcal{Q}$ (see Lemma 4.3). Then $(v, \mathcal{T}_w v)$ corresponds to a solution to (4.1), (4.2). Now we give the detailed proof.

Lemma 4.1. *We presume assumptions* (A1)–(A6). *Then for all* $\widehat{v} \in W^2 + v^D$ *there is exactly one solution to* (4.3). *Moreover,* $\|\mathcal{T}_w\widehat{v}\|_{C(S,Y^4)} \le c$ *for all* $\widehat{v} \in W^2{+}v^D$ *and*

$$\|\mathcal{T}_w\widehat{v}^1 - \mathcal{T}_w\widehat{v}^2\|_{C(S,Y^4)} \le c\left\{\|\widehat{v}^1 - \widehat{v}^2\|_{L^2(S,Y^2)} + \sum_{\gamma=\alpha,\beta}\|\widehat{v}^{1\gamma} - \widehat{v}^{2\gamma}\|_{L^2(S,L^2(\Gamma)^2)}\right\}$$

*for all* $\widehat{v}^1$, $\widehat{v}^2 \in W^2{+}v^D$.

*Proof.* Since for $w \in L^2(S, Y^4)$ the map $w \mapsto \mathcal{R}_w(\widehat{v}, w)$ is Lipschitz continuous uniformly w.r.t. $\widehat{v}$, by [7, Chap. V, Theorem 1.3], problem (4.3) has a unique solution $w = \mathcal{T}_w\widehat{v}$ with a solution operator $\mathcal{T}_w\colon W^2 + v^D \to H^1(S, Y^4)$. Since a.e. on $S$

$$\begin{aligned}&\|\mathcal{R}_w(\widehat{v}^1, w^1) - \mathcal{R}_w(\widehat{v}^2, w^2)\|_{Y^4}\\ &\quad\le c\left(\|\widehat{v}^1 - \widehat{v}^2\|_{Y^2} + \sum_{\gamma=\alpha,\beta}\|\widehat{v}^{1\gamma} - \widehat{v}^{2\gamma}\|_{L^2(\Gamma)^2} + \|w^1 - w^2\|_{Y^4}\right)\end{aligned}$$

for all $(\widehat{v}^1, w^1)$, $(\widehat{v}^2, w^2) \in L^2(S, X)$ we derive by testing (4.3) (for $(\widehat{v}^1, w^1)$ and $(\widehat{v}^2, w^2)$) by $w^1 - w^2$ and by using Gronwall's lemma the Lipschitz-estimate stated in Lemma 4.1. Testing (4.3) by $w = \mathcal{T}_w\widehat{v}$, taking into account that $\rho_M(u) = 0$ for $u$ with $|u|_\infty > M$, and again using Gronwall's lemma the uniform estimate for $\|\mathcal{T}_w\widehat{v}\|_{C(S,Y^4)}$ results. ∎

Lemma 4.2. *We assume assumptions* (A1)–(A6). *Then the mapping* $\mathcal{Q}\colon W^2 + v^D \to W^2 + v^D$ *is completely continuous.*

*Proof.* Let $\{\widehat{v}_n\} \subset W^2 + v^D$ be bounded. According to [16, Theorem 5.1] and (A.1) we may assume that there exists an element $\widehat{v} \in W^2 + v^D$ such that $\widehat{v}_n \to \widehat{v}$ in $L^2(S, Y^2)$, $\widehat{v}_n^\gamma \to \widehat{v}^\gamma$ in $L^2(S, L^2(\Gamma)^2)$, $\gamma = \alpha, \beta$. Let

$$v_n = \mathcal{Q}\widehat{v}_n, \quad v = \mathcal{Q}\widehat{v}, \quad w_n = \mathcal{T}_w\widehat{v}_n, \quad w = \mathcal{T}_w\widehat{v}, \quad z_n = \mathcal{T}_z(\widehat{v}_n, w_n), \quad z = \mathcal{T}_z(\widehat{v}, w).$$

Lemmas 4.1 and 3.1 ensure the convergences $w_n \to w$ in $L^2(S,Y^4)$ and $z_n - z \to 0$ in $L^2(S,Z)$. Testing (4.4) for $\widehat{v}_n$ and $\widehat{v}$ by $v_n - v \in L^2(S, X^2)$ result for $t \in S$,

$$\begin{aligned}&\frac{1}{2}\|(v_n - v)(t)\|_{Y^2}^2 + \int_0^t \epsilon\|v_n - v\|_{X^2}^2\,\mathrm{d}s\\ &\quad\le c\int_0^t \left\{\int_\Omega \sum_{i=1}^2 |[\sigma_M(\widehat{v}_{ni})]^+ - [\sigma_M(\widehat{v}_i)]^+||\nabla z|\,|\nabla(v_{ni} - v_i)|\,\mathrm{d}x\right.\end{aligned}$$

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

$$+\sum_{i=1}^{2}\int_\Omega |\nabla(z_n-z)||\nabla(v_{ni}-v_i)|\,\mathrm{d}x$$
$$+\left(\|\widehat{v}_n-\widehat{v}\|_{Y^2}+\sum_{\gamma=\alpha,\beta}\|\widehat{v}_n^\gamma-\widehat{v}^\gamma\|_{L^2(\Gamma)^2}+\|w_n-w\|_{Y^4}\right)\|v_n-v\|_{X^2}\Bigg\}\,\mathrm{d}s.$$

By Hölder's inequality and Lemma 4.1 we conclude that

$$\begin{aligned}&\|v_n-v\|^2_{L^2(S,X^2)}\\ &\quad\le c\|v_n-v\|_{L^2(S,X^2)}\Bigg\{\|\widehat{v}_n-\widehat{v}\|_{L^2(S,Y^2)}+\sum_{\gamma=\alpha,\beta}\|\widehat{v}_n^\gamma-\widehat{v}^\gamma\|_{L^2(S,L^2(\Gamma)^2)}\\ &\qquad+\|z_n-z\|_{L^2(S,Z)}+\sum_{i=1}^{2}\left[\int_0^T\int_\Omega|[\sigma_M(\widehat{v}_{ni})]^+-[\sigma_M(\widehat{v}_i)]^+|^2\,|\nabla z|^2\,\mathrm{d}x\,\mathrm{d}s\right]^{1/2}\Bigg\}.\end{aligned}$$

Properties of superposition operators give that the square bracket term in the last line tends to zero if $n\to\infty$. Finally, we find that $v_n-v\to 0$ in $L^2(S,X^2)$. Next, we estimate

$$\begin{aligned}&\|(v_n-v)'\|_{L^2(S,X^{2*})}\\ &\quad\le\|\mathcal{R}_v(\widehat{v}_n,w_n)-\mathcal{R}_v(\widehat{v},w)\|_{L^2(S,X^{2*})}+\|\mathcal{A}_v^0(v_n-v)\|_{L^2(S,X^{2*})}\\ &\qquad+\|\mathcal{A}_v(\widehat{v}_n,z_n)-\mathcal{A}_v(\widehat{v},z)\|_{L^2(S,X^{2*})}\\ &\quad\le c\Bigg\{\|v_n-v\|_{L^2(S,X^2)}+\|\widehat{v}_n-\widehat{v}\|_{L^2(S,Y^2)}+\sum_{\gamma=\alpha,\beta}\|\widehat{v}_n^\gamma-\widehat{v}^\gamma\|_{L^2(S,L^2(\Gamma)^2)}\\ &\qquad+\|w_n-w\|_{L^2(S,Y^4)}+\|z_n-z\|_{L^2(S,Z)}\\ &\qquad+\sum_{i=1}^{2}\left[\int_0^T\int_\Omega|[\sigma_M(\widehat{v}_{ni})]^+-[\sigma_M(\widehat{v}_i)]^+|^2\,|\nabla z|^2\,\mathrm{d}x\,\mathrm{d}s\right]^{1/2}\Bigg\}\to 0\end{aligned}$$

for $n\to\infty$, and we obtain $v_n-v\to 0$ in $W^2$. The continuity of the operator $\mathcal{Q}$ follows by similar arguments. ∎

LEMMA 4.3. *We presume assumptions* (A1)–(A6)*. Then there exists a fixed point of the mapping* $\mathcal{Q}$.

*Proof.* For given $\widehat{v}\in W^2+v^D$, let $z=\mathcal{T}_z(\widehat{v},\mathcal{T}_w\widehat{v})$ and $v=\mathcal{Q}\widehat{v}$. We use $\bar{v}:=v-v^D$ as test function for (4.4), take into account assumptions (A4), (A5), and (A6) and use for $\mathcal{R}_v$ that $\rho_M(u)=0$ if $|u|_\infty>M$ and apply (A.1), Lemmas 3.1 and 4.1, and Young's inequality. Then, since $\|\mathcal{T}_z(\widehat{v},\mathcal{T}_w\widehat{v})\|_{H^1}\le c\,(1+\|\widehat{v}-v^D\|_{Y^2})$ we find

$$\begin{aligned}&\|\bar{v}(t)\|^2_{Y^2}+\epsilon\int_0^t\|\bar{v}\|^2_{X^2}\,\mathrm{d}s\\ &\le c+c\int_0^t\left(1+\|\bar{v}\|^2_{Y^2}+\sum_{\gamma=\alpha,\beta}\|\bar{v}^\gamma\|^2_{L^2(\Gamma)^2}+(1+\|z\|_{H^1})\|\bar{v}\|_{X^2}\right)\mathrm{d}s\\ &\le c+\int_0^t\left(\tfrac{\epsilon}{2}\|\bar{v}\|^2_{X^2}+c\left(1+\|\bar{v}\|^2_{Y^2}+\|\widehat{v}-v^D\|^2_{Y^2}\right)\right)\mathrm{d}s\quad\forall t\in S.\end{aligned}$$

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Thus there is a constant $\bar c > 0$ such that for all $k > 0$ the estimate

$$\begin{aligned}
&\mathrm{e}^{-kt}\left(\|\bar v(t)\|_{Y^2}^2 + \int_0^t \|\bar v\|_{X^2}^2\,\mathrm{d}s\right)\\
&\le \bar c + \bar c\mathrm{e}^{-kt}\int_0^t \left\{\left\{\|\bar v\|_{Y^2}^2 + \|\widehat v - v^D\|_{Y^2}^2 + \int_0^s \left(\|\bar v\|_{X^2}^2 + \|\widehat v - v^D\|_{X^2}^2\right)\mathrm{d}\tau\right\}\mathrm{e}^{-ks}\mathrm{e}^{ks}\right\}\mathrm{d}s\\
&\le \bar c + \bar c\mathrm{e}^{-kt}\sup_{s\in S}\left\{\mathrm{e}^{-ks}\left\{\|\bar v(s)\|_{Y^2}^2 + \|\widehat v(s) - v^D\|_{Y^2}^2 + \int_0^s \left(\|\bar v\|_{X^2}^2 + \|\widehat v - v^D\|_{X^2}^2\right)\mathrm{d}\tau\right\}\right\}\frac{\mathrm{e}^{kt}-1}{k}
\end{aligned}$$

holds true. We take now $k \ge 3\bar c$ and obtain

$$\begin{aligned}
&\sup_{t\in S}\mathrm{e}^{-kt}\left(\|\bar v(t)\|_{Y^2}^2 + \int_0^t \|\bar v(s)\|_{X^2}^2\,\mathrm{d}s\right)\\
&\qquad\le \frac{3}{2}\bar c + \frac{1}{2}\sup_{t\in S}\left\{\mathrm{e}^{-kt}\left(\|\widehat v(t) - v^D\|_{Y^2}^2 + \int_0^t \|\widehat v(s) - v^D\|_{X^2}^2\,\mathrm{d}s\right)\right\}.
\end{aligned}$$

Once more using for the reaction terms that $\rho_M(u) = 0$ for $|u|_\infty > M$, and again applying Lemmas 3.1 and 4.1 we estimate

$$\begin{aligned}
&\|\bar v'\|_{L^2(S,X^{2*})} = \sup_{\|\widetilde v\|_{L^2(S,X^2)}\le 1}\langle -\mathcal{R}_v(\widehat v, \mathcal{T}_w\widehat v) - \mathcal{A}_v^0(\bar v) - \mathcal{A}_v(\widehat v, z), \widetilde v\rangle_{L^2(S,X^2)}\\
&\le c\left(\|\bar v\|_{L^2(S,X^2)} + \|z\|_{L^2(S,H^1)} + \|\widehat v - v^D\|_{L^2(S,Y^2)} + 1\right)\\
&\le c\left(\|\bar v\|_{L^2(S,X^2)} + \|\widehat v - v^D\|_{L^2(S,Y^2)} + 1\right)\\
&\le \widetilde c\left(\|\bar v\|_{L^2(S,X^2)} + \left[\sup_{t\in S}\left\{\mathrm{e}^{-kt}\left(\|\widehat v(t) - v^D\|_{Y^2}^2 + \int_0^t \|\widehat v(s) - v^D\|_{X^2}^2\,\mathrm{d}s\right)\right\}\mathrm{e}^{kT}\right]^{1/2} + 1\right).
\end{aligned}$$

The nonempty, bounded, closed, and convex subset of $W^2 + v^D$,

$$\begin{aligned}
\mathcal{M} := \Big\{ v \in W^2 + v^D\colon\ &\sup_{t\in S}\left\{\mathrm{e}^{-kt}\left(\|\bar v(t)\|_{Y^2}^2 + \int_0^t \|\bar v\|_{X^2}^2\,\mathrm{d}s\right)\right\} \le 3\bar c,\\
&\|\bar v'\|_{L^2(S,X^{2*})} \le \widetilde c\left(2\sqrt{3\bar c\mathrm{e}^{kT}} + 1\right)\Big\}
\end{aligned}$$

possesses the property that $\mathcal{Q}(\mathcal{M}) \subset \mathcal{M}$. Since $\mathcal{Q}$ by Lemma 4.2 is completely continuous the assertion of Lemma 4.3 is guaranteed by Schauder's fixed point theorem. □

THEOREM 4.4. *We presume assumptions* (A1)–(A6). *Then there exists a solution* $(u, z)$ *to problem* $(\mathrm{P}_M)$.

*Proof.* Due to Lemma 4.3 there exists a solution $v$ of the problem

$$\begin{aligned}
(v - v^D)' + \mathcal{A}_v^0(v - v^D) &= -\mathcal{R}_v(v, \mathcal{T}_w v) - \mathcal{A}_v(v, \mathcal{T}_z(v, \mathcal{T}_w v)),\\
(v - v^D)(0) &= (U_1, U_2) - v^D, \quad v - v^D \in W^2.
\end{aligned}$$

Putting $w = \mathcal{T}_w v \in H^1(S, Y^4)$, the pair $(v, w)$ fulfills (4.1) and (4.2), which are an equivalent formulation of problem $(\mathrm{P}_M)$. □

**4.3. Energy estimates for $(\mathbf{P}_M)$.** All estimates in this subsection are independent of $M$.

LEMMA 4.5. *We presume assumptions* (A1)–(A6). *Then, for any solution* $(u, z)$ *to* $(\mathrm{P}_M)$ *and for every* $t \in S$ *the inequalities* $u_i(t) \ge 0$ *a.e. on* $\Omega$, $i = 1, 2$, $u_i(t) \in [0, 1]$ $\mu$*-a.e. in* $G$, $i = 3, 4$, $u_{\Gamma i}(t) \in [0, 1]$ $\mu_\Gamma$*-a.e. in* $G_\Gamma$, $i = 1, 2$, *are fulfilled.*

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

*Proof.* Let $(u,z)$ be a solution to $(\mathrm{P}_M)$. We use the test function $-u^-$. Taking into account that

$$(\nabla u_i + \lambda_i[\sigma_M(u_i)]^+\nabla z)\cdot\nabla u_i^- \le 0, \quad -G_{phot}u_i^- \le 0, \quad i=1,2,$$
$$(u_1^+u_2^+ - k_0)(u_1^- + u_2^-) \le 0 \quad \text{a.e. on } \Omega;$$

$$(u_1^+u_4^+ - k_1u_3^+)(u_1^- + u_4^- - u_3^-) \le 0,$$
$$(u_2^+u_3^+ - k_2b_4^+)(u_2^- + u_3^- - u_4^-) \le 0 \quad \mu\text{-a.e. on } G;$$

$$(u_1^{\gamma+}u_{\Gamma 2}^+ - k_{\Gamma 1}u_{\Gamma 1}^+)(u_1^{\gamma-} + u_{\Gamma 2}^- - u_{\Gamma 1}^-) \le 0,$$
$$(u_2^{\gamma+}u_{\Gamma 1}^+ - k_{\Gamma 2}u_{\Gamma 2}^+)(u_2^{\gamma-} + u_{\Gamma 1}^- - u_{\Gamma 2}^-) \le 0 \quad \mu_\Gamma\text{-a.e. on } G_\Gamma \quad \gamma=\alpha,\beta;$$

$$(\sigma_i^\alpha u_i^{\alpha+} - \sigma_i^\beta u_i^{\beta+})(u_i^{\alpha-} - u_i^{\beta-}) \le 0 \quad \text{a.e. on } \Gamma, \quad i=1,2,$$

we find that $\|u^-(t)\|_Y^2 \le 0$ for all $t \in S$. We now argue as in the proof of Lemma 3.2 to verify the remaining results of Lemma 4.5. ∎

We work with a regularized free energy functional $F_M^0$ which is compatible with the regularizations done in problem $(\mathrm{P}_M)$. Let $\delta$ fulfill (3.6). Writing for quantities $y$, the expression $y^\delta := \max\{y,\delta\}$, and using the function

$$l_M(y) = \begin{cases} \ln y & \text{if } \ 0 < y \le M, \\ \ln M - 1 + \frac{y}{M} & \text{if } \ y > M, \end{cases}$$

we introduce the functionals $\widetilde{F}_{M2}^\delta : Y \to \bar{\mathbb{R}}$ by

$$\widetilde{F}_{M2}^\delta(u) = \int_\Omega \sum_{i=1}^2 \int_{u_i^D}^{u_i} (l_M(y^\delta) - \ln u_i^D)\,\mathrm{d}y\,\mathrm{d}x + \sum_{i=3}^4 \int_G \int_{\widetilde{u}_i}^{u_i} (l_M(y^\delta) - \ln \widetilde{u}_i)\,\mathrm{d}y\,\mathrm{d}\mu$$
$$+ \sum_{i=1}^2 \int_{G_\Gamma} \int_{\widetilde{u}_{\Gamma i}}^{u_{\Gamma i}} (l_M(y^\delta) - \ln \widetilde{u}_{\Gamma i})\,\mathrm{d}y\,\mathrm{d}\mu_\Gamma \quad \text{if } u \in Y_+,$$

and $\widetilde{F}_{M2}^\delta(u) = +\infty$ for $u \in Y \setminus Y_+$. Additionally, we set

$$F_{M2}^\delta = (\widetilde{F}_{M2}^{\delta *}|_X)^* : X^* \to \bar{\mathbb{R}}, \quad F_M^\delta = F_1 + F_{M2}^\delta : X^* \to \bar{\mathbb{R}},$$

with $F_1$ from subsection 3.1. Note that the function $l_M$ has the same essential properties as the ln-function occurring in the definitions of $F_2$ and that for $u \in Y$ we have $F_{M2}^\delta(u) \to F_{M2}^0(u)$ and $F_M^\delta(u) \to F_M^0(u)$ as $\delta \downarrow 0$, where $F_{M2}^0(u)$ means $F_{M2}^\delta(u)$ for $\delta = 0$. Especially by the definition of $F_1$ and $l_M$ we have for $u \in Y_+$ and $z$ with $\mathcal{P}(z,u) = 0$ that

$$\|z - z^D\|_Z^2,\ \|u_i \ln u_i\|_{L^1},\ \|u_i\|_{L^1} \le cF_M^0(u) + \widetilde{c}, \quad i=1,2. \tag{4.5}$$

Lemma 4.6. *We presume assumptions* (A1)–(A6). *Let* $(u,z)$ *be a solution to* $(\mathrm{P}_M)$ *and let* $u^\delta = \max\{u,\delta\}$ *for* $\delta < M$ *fulfilling* (3.6). *Then for all* $\tau > 0$ *there exist constants* $c_\tau > 0$, $c > 0$ (*independently on* $M$ *and* $\delta$) *such that*

$$\int_0^t \sum_{\gamma=\alpha,\beta} \left\{ \|\rho_M(u^\delta) r_{\Gamma 1}^\gamma (u_1^\gamma)^\delta (u_{\Gamma 2})^\delta\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)} + \|\rho_M(u^\delta) r_{\Gamma 2}^\gamma (u_2^\gamma)^\delta (u_{\Gamma 1})^\delta\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)} \right\} \mathrm{d}s$$
$$\le c + \int_0^t \left\{ \sum_{i=1}^2 \left\{ \tau \int_\Omega \sigma_M(u_i^\delta) |\nabla l_M(u_i^\delta) + \lambda_i \nabla z|^2\,\mathrm{d}x + c_\tau \|u_i^\delta\|_{L^1(\Omega)} + c\|\nabla(u_i - u_i^\delta)\|_{L^1} \right\} \right.$$
$$\left. + \sum_{+} c(1 + M\delta + \delta^2) \right\} \mathrm{d}s \quad \forall t > 0.$$

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

*Proof.* According to Lemma 4.5 we have $u \geq 0$ for solutions to $(\mathrm{P}_M)$. Similar to the proof of Lemma 3.3, testing in $(\mathrm{P}_M)$ the equations for $u_i$, $i = 1, 2$, on $\Omega^\alpha$ by $\phi^\alpha$, adding them, and leaving out nonnegative terms on the left-hand side, here we obtain

$$\int_0^t \left\{ \int_{G_\Gamma} \rho_M(u)(r^\alpha_{\Gamma 1} u_1^\alpha u_{\Gamma 2} + r^\alpha_{\Gamma 2} u_2^\alpha u_{\Gamma 1})\, \mathrm{d}\mu_\Gamma + \sum_{i=1}^2 \int_\Gamma \rho_M(u)(\sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta)\, \mathrm{d}a \right\} \mathrm{d}s$$
$$\leq \sum_{i=1}^2 \left\{ \|U_i\|_{L^1(\Omega^\alpha)} + \int_0^t \left\{ c + \int_{\Omega^\alpha} \frac{D_i}{\kappa_0} |\nabla u_i + \lambda_i \sigma_M(u_i) \nabla z|\, \mathrm{d}x \right\} \mathrm{d}s \right\} \quad \forall t \in S.$$

Because of $\rho_M(u) = 0$ for $|u|_\infty \geq M$ we find

$$\rho_M(u^\delta)\big[(u_1^\gamma)^\delta (u_{\Gamma 2})^\delta + (u_2^\gamma)^\delta (u_{\Gamma 1})^\delta\big] \leq \rho_M(u)\big[u_1^\gamma u_{\Gamma 2} + u_2^\gamma u_{\Gamma 1}\big] + c(M\delta + \delta^2).$$

Since $\sigma_M(u^\delta) = \sigma_M(u)$ and $\nabla u_i^\delta = \sigma_M(u_i^\delta) \nabla l_M(u_i^\delta)$ we finally estimate the drift-diffusion term using Young's inequality and $\sigma_M(u_i^\delta) \leq u_i^\delta$ by

$$\begin{aligned} |\nabla u_i + \lambda_i \sigma_M(u_i) \nabla z| &\leq |\nabla u_i^\delta + \lambda_i \sigma_M(u_i^\delta) \nabla z| + |\nabla(u_i^\delta - u_i)| \\ &\leq \sigma_M(u_i^\delta) |\nabla l_M(u_i^\delta) + \lambda_i \nabla z| + |\nabla(u_i^\delta - u_i)| \\ &\leq \tau \sigma_M(u_i^\delta) |\nabla l_M(u_i^\delta) + \lambda_i \nabla z|^2 + c_\tau |u_i^\delta| + c|\nabla(u_i - u_i^\delta)|. \end{aligned}$$

This together leads to

$$\int_0^t \Bigg\{ \|\rho_M(u^\delta) r^\alpha_{\Gamma 1} (u_1^\alpha)^\delta (u_{\Gamma 2})^\delta\|_{L^1(G_\Gamma, \mathrm{d}\mu_\Gamma)} + \|\rho_M(u^\delta) r^\alpha_{\Gamma 2} (u_2^\alpha)^\delta (u_{\Gamma 1})^\delta\|_{L^1(G_\Gamma, \mathrm{d}\mu_\Gamma)}$$
$$+ \sum_{i=1}^2 \int_\Gamma \rho_M(u)(\sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta)\, \mathrm{d}a \Bigg\} \mathrm{d}s$$
$$\leq c + \int_0^t \Bigg\{ \sum_{i=1}^2 \left\{ \tau \int_\Omega \sigma_M(u_i^\delta) |\nabla l_M(u_i^\delta) + \lambda_i \nabla z|^2\, \mathrm{d}x + c_\tau \|u_i^\delta\|_{L^1(\Omega)} + c\|\nabla(u_i - u_i^\delta)\|_{L^1} \right\}$$
$$+ c(1 + M\delta + \delta^2) \Bigg\} \mathrm{d}s \quad \forall t \in S.$$

Similar results are obtained by testing the equations for $u_i$, $i = 1, 2$, on $\Omega^\beta$ by $\phi^\beta$, only the term $\int_\Gamma \rho_M(u)(\sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta)\, \mathrm{d}a$ then has the opposite sign. Combining both estimates, the assertion of Lemma 4.6 follows. ∎

LEMMA 4.7. *Under the assumptions* (A1)–(A6) *there exist positive constants* $c_1(T)$, $c_2(T)$ *not depending on* $M$ *such that*

$$F_M^0(u(t)) \leq c_1(T), \quad \|u_i(t) \ln u_i(t)\|_{L^1} \leq c_2(T), \quad i = 1, 2, \quad \forall t \in S$$

*for any solution* $(u, z)$ *to* $(\mathrm{P}_M)$.

*Proof.* Let $(u, z)$ be a solution to $(\mathrm{P}_M)$, let $\delta < M$ fulfill (3.6), and let $u^\delta = \max\{u, \delta\}$. Then $u \in H^1(S, X^*)$, $u \geq 0$, $z - z^D \in L^2(S, Z)$,

$$w_M^\delta := \Big( \big(l_M(u_i^\delta) - \ln u_i^D\big)_{i=1,2}, \big(l_M(u_i^\delta) - \ln \widetilde{u}_i\big)_{i=3,4}, \big(l_M(u_{\Gamma i}^\delta) - \ln \widetilde{u}_{\Gamma i}\big)_{i=1,2} \Big) \in L^2(S, X),$$

and $\lambda(z(t) - z^D) \in \partial F_1(u(t))$, $w_M^\delta(t) \in \partial F_{M2}^\delta(u(t))$ f.a.a. $t \in S$ (note that $l_M(u_i^\delta) = \ln u_i^D$ a.e. on $S \times \Gamma_D$, $i = 1, 2$, and by Lemma 4.5 we have $l_M(u_i^\delta) = \ln u_i^\delta$, $i = 3, 4$,

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

$l_M(u^\delta_{\Gamma i}) = \ln(u^\delta_{\Gamma i})$, $i = 1, 2$). Thus, according to Lemma A.1, we get for $\zeta^\delta_M := w^\delta_M + \lambda(z - z^D)$ that

$$\begin{aligned}
&\big[F_1(u(t)) + F^\delta_{M2}(u(t))\big]\Big|_0^t \\
&\qquad = \int_0^t \langle u'(s), \zeta^\delta_M(s)\rangle_X \,\mathrm{d}s \\
&\qquad = -\int_0^t \langle \mathcal{R}_M(u(s)) + \mathcal{A}_M(u(s), z(s)), \zeta^\delta_M(s)\rangle_X \,\mathrm{d}s \\
&\qquad = -\int_0^t \big\{\langle \mathcal{R}_M(u^\delta(s)) + \mathcal{A}_M(u^\delta(s), z(s)), \zeta^\delta_M(s)\rangle_X - \theta^\delta(s)\big\}\,\mathrm{d}s,
\end{aligned}$$

where $\theta^\delta = \langle \mathcal{R}_M(u^\delta) - \mathcal{R}_M(u) + \mathcal{A}_M(u^\delta, z) - \mathcal{A}_M(u, z), \zeta^\delta_M\rangle_X \to 0$ for $\delta \downarrow 0$. Since all the reaction terms containing the factor $\rho_M(u^\delta)$ become zero if $|u^\delta|_\infty > M$, we have for these terms only to discuss the situation $u^\delta_i \le M$, and here is $l_M(u^\delta_i) = \ln u^\delta_i$. We arrive at

$$\begin{aligned}
-\langle \mathcal{R}_M(u^\delta), \zeta^\delta_M\rangle_X \le{}& c\left(1 + \sum_{i=1}^2 \|u^\delta_i\|_{L^1}\right)\Big(\|\ln \tfrac{u_1^D u_2^D}{k_0}\|_{L^\infty} + \|\tfrac{k_1 k_2}{u_1^D u_2^D}\|_{L^\infty(G,\mathrm{d}\mu)}\Big) \\
&+ c\,\|G_{phot}\|_{L^\infty}\left\{\sum_{i=1}^2 \big(\|u^\delta_i\|_{L^1} + \|\ln u^D_i\|_{L^1}\big) + \|z - z^D\|_{L^1}\right\} \\
&+ c\,(1 + \|\rho_M(u^\delta) r^\beta_{\Gamma 1}(u^\beta_1)^\delta (u_{\Gamma 2})^\delta\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)})\|\tfrac{k^\beta_{\Gamma 1} u_1^{\alpha D}}{k^\alpha_{\Gamma 1} u_1^{\beta D}}\|_{L^\infty(G_\Gamma,\mathrm{d}\mu_\Gamma)} \\
&+ c\,(1 + \|\rho_M(u^\delta) r^\alpha_{\Gamma 2}(u^\alpha_2)^\delta (u_{\Gamma 1})^\delta\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)})\|\tfrac{k^\alpha_{\Gamma 1} k^\alpha_{\Gamma 2}}{u_1^{\alpha D} u_2^{\alpha D}}\|_{L^\infty(G_\Gamma,\mathrm{d}\mu_\Gamma)} \\
&+ c\,(1 + \|\rho_M(u^\delta) r^\beta_{\Gamma 2}(u^\beta_2)^\delta (u_{\Gamma 1})^\delta\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)})\|\tfrac{k^\alpha_{\Gamma 1} k^\beta_{\Gamma 2}}{u_1^{\alpha D} u_2^{\beta D}}\|_{L^\infty(G_\Gamma,\mathrm{d}\mu_\Gamma)}.
\end{aligned}$$

Observing that on solutions $[\sigma_M(u^\delta_i)]^+ = \sigma_M(u^\delta_i) \le u^\delta_i$, $\nabla l_M(u^\delta_i) = \nabla(u^\delta_i)/\sigma_M(u^\delta_i)$, $i = 1, 2$, using assumptions (A4), (A5), and Young's inequality we find a.e. on $S$ that

$$\begin{aligned}
&-\langle \mathcal{A}_M(u^\delta, z), \zeta^\delta_M\rangle_X \\
&\quad = -\int_\Omega \sum_{i=1}^2 D_i \sigma_M(u^\delta_i)\Big\{|\nabla(l_M(u^\delta_i) + \lambda_i z)|^2 - \nabla(l_M(u^\delta_i) + \lambda_i z)\cdot\nabla(\ln u^D_i - \lambda_i z^D)\Big\}\,\mathrm{d}x \\
&\quad \le \sum_{i=1}^2 \left(c\|u^\delta_i\|_{L^1}\|\nabla(\ln u^D_i + \lambda_i z^D)\|^2_{L^\infty} - \tfrac{\epsilon}{2}\int_\Omega \sigma_M(u^\delta_i)|\nabla(l_M(u^\delta_i) + \lambda_i z)|^2\,\mathrm{d}x\right).
\end{aligned}$$

Putting both estimates together, using Lemma 4.6, taking $\delta \downarrow 0$ in the previous three estimates, and using assumptions (A3) and (A5), and (4.5), we arrive at

$$F^0_M(u(t)) - F^0_M(U) \le c\int_0^t (1 + F^0_M(u(s)))\,\mathrm{d}s,$$

where $c$ depends on the data, but not on $M$. Due to the choice of $M$ we have $F^0_M(U) = F(U)$. By Gronwall's lemma we obtain the first assertion of Lemma and the last result of the lemma follows by (4.5). ∎

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

**4.4. Further estimates for $(\mathbf{P}_M)$.** The estimates in this subsection are independent of $M$.

THEOREM 4.8. *Under the assumptions* (A1)–(A6) *there is a constant* $c^*(T) > 0$ *not depending on* $M$ *such that for any solution* $(u, z)$ *to* $(\mathrm{P}_M)$,

$$\|u\|_{L^\infty(S,V)} \le c^*(T). \tag{4.6}$$

*Proof.* 1. Let $q > 2, r$, and $r'$ be chosen as in Lemma 3.2 (ii) and (3.3) and let $(u, z)$ be a solution to $(\mathrm{P}_M)$. By Lemma 4.5 and Lemma 3.2 (ii) it follows

$$\|z(t)\|_{W^{1,q}} \le c\Big[1 + \textstyle\sum_{i=1,2} \|u_i(t)\|_{L^{r'}}\Big] \quad \forall t \in S. \tag{4.7}$$

2. Let $v_i = (u_i - \hat{K})^+$, $i = 1, 2$, where $\hat{K}$ is given in (3.8). We test $(\mathrm{P}_M)$ by $2(v_1, v_2, 0, 0, 0, 0)$. Estimating $[\sigma_M(u_i)]^+$ by $v_i + \hat{K}$, using Lemma 4.5, (4.7), (A.2), the trace inequality (A.1), Young's inequality, Lemma 4.7, and (4.5) we obtain

$$\begin{aligned}
\sum_{i=1,2} \|v_i(t)\|_{L^2}^2 \le \int_0^t \sum_{i=1,2} \Bigg\{ &- 2\epsilon \|v_i\|_{H^1}^2 + c \Bigg( \|v_i\|_{L^r} \|z\|_{W^{1,q}} \|v_i\|_{H^1} + \|z\|_{H^1} \|v_i\|_{H^1} \\
&+ \|v_i\|_{L^2}^2 + \sum_{\gamma=\alpha,\beta} \|v_i^\gamma\|_{L^2(\Gamma)}^2 + 1 \Bigg) \Bigg\} \,\mathrm{d}s \\
\le \int_0^t \sum_{i=1,2} \Bigg\{ &-\epsilon \|v_i\|_{H^1}^2 + \bar{c} \|v_i\|_{L^r} \|v_i\|_{H^1} \sum_{k=1,2} \|v_k\|_{L^{r'}} + c \Bigg\} \,\mathrm{d}s.
\end{aligned}$$

By $\|v_k\|_{L^{r'}} \le \|v_k\|_{L^1}^{(r-2)/r} \|v_k\|_{L^2}^{2/r}$, by inequality (A.3) for $p = 2$ and by Lemma 4.7 we get

$$\begin{aligned}
\bar{c} \sum_{i=1,2} \|v_i\|_{L^r} \|v_i\|_{H^1} \sum_{k=1,2} \|v_k\|_{L^{r'}} &\le \sum_{i=1,2} \Bigg\{ \frac{\epsilon}{2} \|v_i\|_{H^1}^2 + c \|v_i\|_{L^2}^2 \sum_{k=1,2} \|v_k\|_{L^2}^2 \Bigg\} \\
\le \sum_{i=1,2} \Bigg\{ \frac{\epsilon}{2} \|v_i\|_{H^1}^2 &+ \Big[ \frac{\sqrt{\epsilon}}{2c_2(T)} \|v_i \ln v_i\|_{L^1} \|v_i\|_{H^1} + c \|v_i\|_{L^1} \Big]^2 \Bigg\} \le \sum_{i=1,2} \epsilon \|v_i\|_{H^1}^2 + c.
\end{aligned}$$

By the previous estimates and inequality (4.7) we find positive constants $c(T)$, $\widetilde{\kappa}$ independent of $M$ such that

$$\|v_i(t)\|_{L^2} \le c(T)\,, \ i = 1, 2, \quad \|z(t)\|_{W^{1,q}}^{2r} + 1 \le \widetilde{\kappa}(T) \quad \forall t \in S. \tag{4.8}$$

3. Similar to the estimates in the proof of Theorem 3.6, but estimating $[\sigma_M(u_i)]^+$ by $v_i + \hat{K}$ and using $\widetilde{\kappa}(T)$ from (4.8) instead of $\kappa$, we can verify that $\|v_i(t)\|_{L^\infty} \le c(T)$ for all $t \in S$, which leads to the desired upper bounds for $u_i$, $i = 1, 2$, on $S$. Since by Lemma 4.5 the quantities $u_3$, $u_4$, $u_{\Gamma 1}$, and $u_{\Gamma 2}$ lie in $[0, 1]$ for all $t \in S$, the proof is done. ∎

**4.5. Existence and uniqueness result for (P).** Now we are ready to prove the main results of the paper.

THEOREM 4.9. *We presume assumptions* (A1)–(A6). *Then there exists at least one solution to* (P).

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

*Proof.* Note that it is sufficient to show the existence of a solution to (P) on any finite time interval $S = [0, T]$. We call such problems ($\mathrm{P}_S$) and choose the regularization level $\bar{M} = 2\,c^*(T)$ (see Theorem 4.8). Then Theorem 4.4 guarantees a solution $(u, z)$ to ($\mathrm{P}_{\bar{M}}$). The choice of $\bar{M}$ ensures that the operators $\mathcal{R}_{\bar{M}}$ and $\mathcal{R}$ as well as the operators $\mathcal{A}_{\bar{M}}$ and $\mathcal{A}$ coincide on this solution. Therefore, $(u, z)$ is a solution to ($\mathrm{P}_S$), too. □

THEOREM 4.10. *Under the assumptions* (A1)–(A6) *the solution to* (P) *is unique.*

*Proof.* We prove uniqueness on every finite time interval $S := [0, T]$. Let $(u^k, z^k)$, $k = 1, 2$, be two solutions to (P). We find a constant $c > 0$ such that $\|u^k(t)\|_V$, $\|\nabla z^k(t)\|_{L^q} \le c$ f.a.a. $t \in S$, $k = 1, 2$, where $q > 2$ (see Lemma 3.2 ii), too). Let $\bar{u} := u^1 - u^2$, $\bar{z} := z^1 - z^2$. According to (3.1) we obtain

$$\|\bar{z}(t)\|_{H^1} \le c\|\bar{u}(t)\|_Y \qquad \text{f.a.a. } t \in S. \tag{4.9}$$

We test (P) by $\bar{u} \in L^2(S, X)$ and take into account Lemma 3.2 (i) and the fact that the reaction rates are uniformly locally Lipschitz continuous in the state variable. With the Gagliardo–Nirenberg inequality $\|\bar{u}_i\|_{L^r(\Omega^\gamma)} \le \|\bar{u}_i\|^{2/r}_{L^2(\Omega^\gamma)} \|\bar{u}_i\|^{1-2/r}_{H^1(\Omega^\gamma)}$, $i = 1, 2$, $\gamma = \alpha, \beta$, for $r$ from (3.3), with inequality (4.9), the trace inequality (A.1) for $\|\bar{u}_i^\gamma\|^2_{L^2(\Gamma)}$, and with Young's inequality we conclude as follows:

$$\begin{aligned}
&\tfrac{1}{2}\|\bar{u}(t)\|_Y^2 + \sum_{i=1,2} \int_0^t \epsilon \|\bar{u}_i\|^2_{H^1} \mathrm{d}s \\
&\le c \int_0^t \left\{ \sum_{i=1}^2 \left\{ \|\bar{u}_i\|_{L^r} \|\nabla z^1\|_{L^q} \|\nabla \bar{u}_i\|_{L^2} + \|\nabla \bar{z}\|_{L^2} \|\nabla \bar{u}_i\|_{L^2} + \sum_{\gamma=\alpha,\beta} \|\bar{u}_i^\gamma\|^2_{L^2(\Gamma)} \right\} \right\} \mathrm{d}s \\
&\quad + c \int_0^t \|\bar{u}\|_Y^2 \,\mathrm{d}s \\
&\le \int_0^t \left\{ \sum_{i=1}^2 \left\{ \tfrac{\epsilon}{4} \|\bar{u}_i\|^2_{H^1} + c\|\bar{u}_i\|^{2/r}_{L^2} \|\nabla z^1\|_{L^q} \|\bar{u}_i\|^{2-2/r}_{H^1} \right\} + c\|\bar{u}\|_Y^2 \right\} \mathrm{d}s \\
&\le \int_0^t \left\{ \sum_{i=1}^2 \left\{ \tfrac{\epsilon}{2} \|\bar{u}_i\|^2_{H^1} + c\|\nabla z^1\|^r_{L^q} \|\bar{u}_i\|^2_{L^2} \right\} + c\|\bar{u}\|_Y^2 \right\} \mathrm{d}s \\
&\le \int_0^t \left\{ \sum_{i=1}^2 \tfrac{\epsilon}{2} \|\bar{u}_i\|^2_{H^1} + c\|\bar{u}\|_Y^2 \right\} \mathrm{d}s \quad \forall t \in S.
\end{aligned}$$

Therefore Gronwall's lemma leads to $\bar{u} = 0$ on $S$, and (4.9) completes the proof. □

**5. Remarks and generalizations of the results of this paper.** 1. In this paper we studied the simplest situation of a heterostructure $\Omega$ with active interface as indicated in Figure 1.1 consisting of two materials $\Omega^\alpha$ and $\Omega^\beta$ and an active interface $\Gamma$ in between. The presented results can easily be generalized to the situation of multimaterial-heterostructures with several active interfaces. But for the analytic treatment we need that active interfaces and the parts of the boundary of $\Omega$, where Dirichlet boundary conditions are prescribed, are strictly separated (see Lemmas 3.3 and 4.6).

2. In this paper we restricted for an easier writing to the case of exactly one kind of trap in the volume and one kind of trap at the interface. The results of this paper remain true, if different kinds of traps (in possibly different subdomains) and

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

different kinds of traps on interfaces are considered. Such models are presented in [20], there are the one-dimensional simulation tool AFORS-HET for the simulation of solar cells and solar cell characterization methods introduced. Especially in solar cells with polycrystalline materials, there occur simultaneously acceptor like and donator like traps at grain boundaries which have Gaussian like profiles with respect to their energy distribution where both profiles are slightly shifted against each other.

3. In the present model we studied drift-diffusion processes in subdomains which are coupled by an active interface $\Gamma$. In comparison to the situation in [9], we now study nontrivial transfer conditions at $\Gamma$ involving thermionic emission and capture and release of charge carriers by immobile interfacial traps. Thus additional ODEs for the energy resolved traps at the interface have to be included in the model. Note that the Poisson equation is still formulated on the whole domain $\Omega$ but now containing an extra source term at the interface $\Gamma$ resulting from charged interface traps. In the considered physical situation it is not justified to have simultaneous equilibrium of all considered processes. In comparison to the techniques in [9] now in the a priori estimates and the existence proof, a lot of additional terms have to be managed. Pariticulary, Lemma 3.3 is needed to prove the energy estimates.

4. The assumption $\Omega \subset \mathbb{R}^2$ supplies (due to [13]) sufficient regularity of the solution to the Poisson equation (cf. Lemma 3.2) to manage the drift terms in the a priori estimates which fails in the situation of higher spatial dimensions. Especially in the two-dimensional situation the Gagliardo–Nirenberg inequality fits well to estimate the source terms in Lemma 3.5 and Theorem 3.6, which is not given in the three-dimensional situation. The situation is comparable to that of the classical van Roosbroeck system and of problems in semiconductor technology; see [6, 10]. The situation becomes easier in the case of pure reaction-diffusion systems.

5. Of course also volume or interface traps which can be occupied by multiple charge carriers can be treated by our technique. We then would have to use charge numbers appropriate for this situation and would have to introduce additional ionization reactions.

6. The authors of [11] presented a (formal) generalized gradient flow formulation for electro-reaction-diffusion systems on heterostructures and with active interfaces. This paper is an extension of the ideas in [17] to heterostructures and to active interfaces, where at interfaces the following effects are taken into account: drift-diffusion processes and reactions of species living on the interface and transfer mechanisms allowing bulk species to pass the interface.

For the case of closed systems the equations discussed in the present paper can be written as a generalized gradient flow, too, provided that the rate coefficients of the generation/recombination of electrons and holes $k_0$, of the bulk ionization reactions $k_i$, of the ionization reactions at the interface $k^\gamma_{\Gamma i}$ and the coefficients $\sigma^\gamma_i$ in the thermionic emission interface condition, $i = 1, 2$, $\gamma = \alpha, \beta$, fulfill Wegscheider conditions allowing for detailed balance of the reactions under consideration. Have in mind that in our notation the transfer coefficients $\sigma^\gamma_i$ are incorporated in the boundary value functions $u^{\gamma D}_i$ (see assumption (A5)).

**Appendix.** Let $\Omega \subset \mathbb{R}^2$ be a bounded Lipschitzian domain. We use Sobolev's imbedding results (see [15]) and the following trace inequality, which can be derived from [15, eq. 5, p. 317] by a modified application of Hölder's inequality

$$\|w\|^q_{L^q(\partial\Omega)} \le c_\Omega\, q \|w\|^{q-1}_{L^{2(q-1)}(\Omega)} \|w\|_{H^1(\Omega)} \quad \forall w \in H^1(\Omega), \quad q \ge 2. \tag{A.1}$$

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Moreover, we take advantage of the Gagliardo–Nirenberg inequality

$$\|w\|_{L^p} \le c_p \, \|w\|_{L^1}^{1/p} \|w\|_{H^1}^{1-1/p} \quad \forall w \in H^1(\Omega)\,,\ 1 < p < \infty \tag{A.2}$$

(see [4, 19]). As an extended version of this inequality one obtains that for any $\delta > 0$ and any $p \in (1, \infty)$ there exists a $c_{\delta,p} > 0$ such that

$$\|w\|_{L^p}^p \le \delta \, \|w \ln |w|\|_{L^1} \, \|w\|_{H^1}^{p-1} + c_{\delta,p} \, \|w\|_{L^1} \quad \forall w \in H^1(\Omega). \tag{A.3}$$

This inequality is verified in [1] for bounded smooth domains and $p = 3$. But (A.3) is true for bounded Lipschitzian domains and $p \in (1, \infty)$, too, since (A.2) is valid in this situation, too. Finally, we make use of the following chain rule, which can be derived from [2, Lemma 3.3].

LEMMA A.1. *Let $X$ be a Hilbert space and let $X^*$ be its dual, $S = [0, T]$. Let $F : X^* \to \bar{\mathbb{R}}$ be proper, convex, and semicontinuous. Assume that $u \in H^1(S, X^*)$, $f \in L^2(S, X)$, and $f(t) \in \partial F(u(t))$ f.a.a. $t \in S$. Then $F \circ u : S \to \mathbb{R}$ is absolutely continuous, and*

$$\frac{\mathrm{d}\,(F \circ u)}{\mathrm{d}t}(t) = \Big\langle \frac{\mathrm{d}u}{\mathrm{d}t}(t), f(t) \Big\rangle_X \quad \textit{f.a.a. } t \in S.$$

## REFERENCES


[1] P. BILER, W. HEBISCH, AND T. NADZIEJA, *The Debye system: Existence and large time behavior of solutions*, Nonlinear Anal., 23 (1994), pp. 1189–1209.

[2] H. BRÉZIS, *Opérateurs maximaux monotones et semi-groups de contractions dans les espaces de Hilbert*, North–Holland Math. Stud. 5, North–Holland, Amsterdam, 1973.

[3] I. EKELAND AND R. TEMAM, *Convex Analysis and Variational Problems*, Stud. Math. Appli. 1, North–Holland, Amsterdam, 1976.

[4] E. GAGLIARDO, *Ulteriori proprietà di alcune classi di funzioni in più variabili*, Ricerche Mat., 8 (1959), pp. 24–51.

[5] H. GAJEWSKI, *Analysis und Numerik von Ladungstransport in Halbleitern (Analysis and numerics of carrier transport in semiconductors)*, Mitt. Ges. Angew. Math. Mech., 16 (1993), pp. 35–57.

[6] H. GAJEWSKI AND K. GRÖGER, *Initial boundary value problems modelling heterogeneous semiconductor devices*, Surveys on Analysis, Geometry and Mathematical, Physics Teubner-Texte Math. 117, B. W. Schulze and H. Triebel, eds., Teubner, Leipzig, 1990, pp. 4–53.

[7] H. GAJEWSKI, K. GRÖGER, AND K. ZACHARIAS, *Nichtlineare Operatorgleichungen und Operatordifferentialgleichungen*, Akademie–Verlag, Berlin, 1974.

[8] A. GLITZKY, *Analysis of a spin-polarized drift-diffusion model*, Adv. Sci. Appl., 18 (2008), pp. 401–427.

[9] A. GLITZKY, *Analysis of electronic models for solar cells including energy resolved defect densities*, Math. Methods Appl. Sci., 34 (2011), pp. 1980–1998.

[10] A. GLITZKY AND R. HÜNLICH, *Global existence result for pair diffusion models*, SIAM J. Math. Anal., 36 (2005), pp. 1200–1225.

[11] A. GLITZKY AND A. MIELKE, *A gradient structure for systems coupling reaction-diffusion effects in bulk and interfaces*, Preprint 1603, Weierstraß-Institut für Angewandte Analysis und Stochastik, Berlin, 2011; Z. Angew. Math. Phys., Submitted.

[12] K. GRÖGER, *Initial-boundary value problems describing mobile carrier transport in semiconductor devices*, Comment. Math. Univ. Carolin., 26 (1985), pp. 75–89.

[13] K. GRÖGER, *A $W^{1,p}$-estimate for solutions to mixed boundary value problems for second order elliptic differential equations*, Math. Ann., 283 (1989), pp. 679–687.

[14] H.-CH. KAISER, H. NEIDHARDT, AND J. REHBERG, *Classical solutions of drift-diffusion equations for semiconductor devices: The two-dimensional case*, Nonlinear Anal., 71 (2009), pp. 1584–1605.

[15] A. KUFNER, O. JOHN, AND S. FUČIK, *Function Spaces*, Academia, Prague, 1977.

[16] J. L. LIONS, *Quelques méthodes de résolution des problèmes aux limites non linéaires*, Dunod, Gauthier-Villars, Paris, 1969.


Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

[17] A. Mielke, *A gradient structure for reaction-diffusion systems and for energy-drift-diffusion systems*, Nonlinearity, 24 (2011), pp. 1329–1346.

[18] M. S. Mock, *An initial value problem from semiconductor device theory*, SIAM J. Math. Anal., 5 (1974), pp. 597–612.

[19] L. Nirenberg, *An extended interpolation inequality*, Ann. Scuola Norm. Sup. Pisa (3), 20 (1966), pp. 733–737.

[20] R. Stangl, C. Leendertz, and J. Haschke, *Numerical simulation of solar cells and solar cell characterization methods: The open-source on demand program AFORS-HET*, Solar Energy, R. D. Rugescu, ed., InTech, Croatia, 2010, pp. 319–352.

[21] W. V. van Roosbroeck, *Theory of the flow of electrons and holes in germanium and other semiconductors*, Bell Syst. Techn. J., 29 (1950), pp. 560–607.

[22] H. Wu, P. A. Markowich, and S. Zheng, *Global existence and asymptotic behavior for a semiconductor drift-diffusion-Poisson model*, Math. Models Methods Appl. Sci., 18 (2008), pp. 443–487.

Downloaded 02/08/19 to 62.141.176.1. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.